Colloquium
We are who we've been waiting for
Greetings!

On behalf of the Director’s Office, it is my pleasure to welcome you to 2017 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 190 participants from 100 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 SURF participants. 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 specific 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 National Institute of Standards and Technology (NIST) Facebook page using the hashtag, #2017SURFColloquium.

Lastly, I could not conclude this letter without mentioning the individuals which make the SURF Program at NIST possible. Thank you to the OU SURF Directors, the SURF mentors, and all the staff at NIST who play an integral role in making the SURF participants experience valuable. Your hard work and dedication to the program is 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
Managing SURF Program Director (NIST-wide)
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## NIST SURF Program Staff by Organizational Unit (OU)

<table>
<thead>
<tr>
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<th>Name</th>
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<tr>
<td>Director’s Office</td>
<td>Brandi Toliver, Managing SURF Program Director</td>
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<tr>
<td>Director’s Office</td>
<td>Kara Arnold</td>
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<tr>
<td>Center for Nanoscale Science and Technology</td>
<td>John Unguris</td>
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<tr>
<td>Center for Nanoscale Science and Technology</td>
<td>Kartik Srinivasan</td>
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<td>Engineering Lab</td>
<td>Lisa Jean Fronczek</td>
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<td>Cartier Murrill</td>
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<td>Lotfi Benmohamed</td>
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<td>Michaela Iorga</td>
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<td>Elizabeth Lennon</td>
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<td>Communications Technology Lab</td>
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<td>Material Measurement Lab</td>
<td>Rebecca Zangmeister</td>
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<td>Material Measurement Lab</td>
<td>Amanda Forster</td>
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<td>Julie Borchers</td>
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<td>Joseph Dura</td>
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<td>Physical Measurement Lab-Electrical Eng</td>
<td>Joseph Kopanski</td>
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<td>Richard Steiner</td>
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<td>Darwin Reyes-Hernandez</td>
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<td>Cameron Miller</td>
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<td>Physical Measurement Lab-Physics Lab</td>
<td>Uwe Arp</td>
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<td>Physical Measurement Lab-Physics Lab</td>
<td>Maritoni Litorja</td>
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<td>Technology Partnership Office</td>
<td>Paul Zielinski</td>
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<td>Standards Coordination Office</td>
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<td>Welcome</td>
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<td><strong>Session Moderator: TBA</strong></td>
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<td>9:15A</td>
<td>CNST</td>
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<td>9:45A</td>
<td>CTL</td>
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<td></td>
<td>Vineet Shenoy: Simulation of SAS-CBSD protocol for CBRS band</td>
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<td>10:15A</td>
<td>EL</td>
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<td></td>
<td>Omar Aboul-Enein: Performance Measurement of Mobile Manipulators: Expansion to Autonomous-Unmanned Ground Vehicles (A-UGVs)</td>
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<td>10:45A</td>
<td>ITL</td>
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<td></td>
<td>Kelsey Fulton: Unwinding the Runtime Stack: Application Runtime Analysis for Anomaly Detection Research</td>
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<td>11:15A</td>
<td>MML</td>
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<td>Alison Farrar: Materials for Magnetic Nanothermometry: Experimental Investigation</td>
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<td>11:45A</td>
<td>NCNR</td>
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<td></td>
<td>Emily Blick: The Role of Detergents in the Crystallization of Membrane Proteins from Lipidic Cubic Phases</td>
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<tr>
<td>12:15P</td>
<td>PML</td>
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<td></td>
<td>Rebecca Moore: My Summer as a Lab Therapist: Fostering Effective Communication between Hardware, Software, and the Physicist</td>
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<tr>
<td>12:45P</td>
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Parallel Sessions: Tuesday, August 1, 2017 (Afternoon)

<table>
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<th>ITL</th>
<th>MML/NCNR MatSci</th>
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<th>PML PL</th>
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</table>
| 2:20P | Andrew Essex: Copper Electrodeposition on a Rotating Disk Electrode: Hydrodynamic Effects on Spatial Patterning in the Presence of a Polymer-Chloride Adlayer

**Cayla Collett:** Quantification of Drugs

**Andrew Ericks:** Copper Electrodeposition on a Rotating Disk Electrode: Hydrodynamic Effects on Spatial Patterning in the Presence of a Polymer-Chloride Adlayer

**Jamie Thorpe:** Construction of 2D and 3D Mageto-Optical Traps for Lithium and Rubidium Atoms

**Lauren Cabrera:** Encrypting CAN Bus Communication Using a Lightweight Cryptographic Algorithm

**Nikita Wootten:** Better Auditing of IoT Devices Through Cryptographic Hash Chaining of Logs and Logcrypt Signing

**Deandra Francis:** Raman and THz Raman Spectroscopy for Forensic application of illicit narcotics and explosives

**Dmitry Leontyev:** Optimization of mini-DART-MS for the Detection of Smokeless Powder Residues

**Adicor Laperio:** First Principles Study of the Energetic Ordering and Phase Stability of High-Energy Density Li-S Batteries by Focused Ion and Electron Beam Techniques

**Ramesses Qucezada:** Fabrication of a Platinum/Gold Dual Electrode for Applications in Electrochemical DNA Sensing

**Richard Torisi:** Latent Fingerprint Development Standards Development

**Chloe Cook:** Single Ion Probe Manipulation and Characterization of Point Defects in Functional Oxide Materials

**Addie Lupercio:** First Principles Study of the Energetic Ordering and Phase Stability of High-Energy Density Li-S Batteries by Focused Ion and Electron Beam Techniques

**Raymond Lin:** IoT Device Identification Using Packet Analysis

**Ramsess Quezada:** Fabrication of a Platinum/Gold Dual Electrode for Applications in Electrochemical DNA Sensing

**Dmitry Leontyev:** Optimization of mini-DART-MS for the Detection of Smokeless Powder Residues

**Edward Arnheiter:** Analyzing Surface Chemistry of Thin Film Platinum via Nanocalorimetry

**Nicole Seese:** Exploring the Utility of the PAQ4 Data Compressor for Estimation of Min-Entropy

**Hionu (Anthony) Chung:** Evaluating Combined Shear and Compression Test Methods for Impact Mitigating Materials

**Tony Allen:** The Use of Graph Theory in Forensic Footwear Analysis

**Ariel Shlosberg:** Revisualization of Thorium Atlas for Calibration of Astronomical Spectrographs

**Xinyu Xiong:** Access Control Rule Logic Circuit Simulation (ACRLCS)

**Nicole Seese:** Exploring the Utility of the PAQ4 Data Compressor for Estimation of Min-Entropy

**Nhi Phan:** Assembly of a Dedicated Quantitative Imager for Fluorescence and Bioluminescence

**Peter Zhou:** Bragg diffraction as a probe of transition to a Bose-Einstein condensate

**Andrew Gayle:** Investigating Atomic Force Microscopy for Forensic Analysis of Hair from Individuals

**Chloe Cook:** Single Ion Probe Manipulation and Characterization of Point Defects in Functional Oxide Materials

**Nicole Seese:** Exploring the Utility of the PAQ4 Data Compressor for Estimation of Min-Entropy

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**Matthew Wade:** Analysis of Polymer Thin Films for Organic Photovoltaics Through In-situ Spectroscopic Ellipsometry, or How I Learned to Watch Paint Dry

**Emily McGovern:** Geometric Characterization of Features for Forensic Footwear Impression Comparisons

**Alexis Brake:** Evaluating the role of fiber degradation in affecting the aging characteristics of carbon nanotube based hierarchical composites

**Matthew Wade:** Analysis of Polymer Thin Films for Organic Photovoltaics Through In-situ Spectroscopic Ellipsometry, or How I Learned to Watch Paint Dry

**Emily McGovern:** Geometric Characterization of Features for Forensic Footwear Impression Comparisons
Parallel Sessions: Wednesday, August 2, 2017 (Morning)

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<tr>
<th>Time</th>
<th>Lecture Room A</th>
<th>MML/NCNR ChemBio</th>
<th>MML/NCNR MatSci</th>
<th>MML/NCNR MML/NCNR PL</th>
<th>ITL EL PML PL</th>
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<tr>
<th>Time</th>
<th>Lecture Room A</th>
<th>Lecture Room B</th>
<th>Lecture Room C</th>
<th>Lecture Room D</th>
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<tr>
<td>1:00P</td>
<td>Characterizing and Control of Nanostructures</td>
<td>Fusing Deposition Manufacturing</td>
<td>Electron Beam Lithography</td>
<td>Chemical Patterning</td>
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<td>Characterizing and Control of Nanostructures</td>
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<td>Characterizing and Control of Nanostructures</td>
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<tr>
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<td>Characterizing and Control of Nanostructures</td>
<td>Fusing Deposition Manufacturing</td>
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<td>Characterizing and Control of Nanostructures</td>
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<td>2:00P</td>
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<td>Chemical Patterning</td>
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**Lecture Room A**
- **Chad Phillips:** Characterizing application of the Materials Resource Registry (NIST)
- **Sai Meghasena Chavali:** Development of 2-Dimensional Nanoelectronic Devices
- **Daniel Oler:** Microfluidic Devices
- **Doua Vang:** Organic Transistors: Devices and Dose
- **Lily Motabar:** Constructing Novel Photonic Sensor Networks

**Lecture Room B**
- **Emma DiBernardo:** Nickel Ion Interactions with Mutant Alphabeta Sensors
- **Suzanna Capric:** Hemolysin Nanopore Interactions with Mutant Alpha-Spectrin
- **Emma Galvani:** Evaluation and Analysis of Machine Learning Algorithms
- **Ananya Srinivasan:** Structuring for Searchable Knowledge: Leveraging the Efficient Searching of the NIST Tandem Mass Spectral Library
- **Sally Jiao:** Predicting Low-Temperature Structural Properties from High-Temperature Molecular Simulations

**Lecture Room C**
- **Shane Regan:** Profiling the Electrical Shape of a KPFM Probe
- **Malcolm Regan:** Profiling the Electrical Shape of a KPFM Probe
- **Doua Vang:** Organic Transistors: Devices and Dose
- **Doua Vang:** Organic Transistors: Devices and Dose
- **Doua Vang:** Organic Transistors: Devices and Dose

**Lecture Room D**
- **Kathleen Mullin:** WebFF Data Project
- **Rachel Devers:** More Accurate Compound Identification in the NIST Tandem Mass Spectral Library
- **Emily Brown:** Enhancing the Process for In-Solution Synthesis of Methylated Alkyl Ketones
- **Sally Jiao:** Predicting Low-Temperature Structural Properties from High-Temperature Molecular Simulations
- **Sally Jiao:** Predicting Low-Temperature Structural Properties from High-Temperature Molecular Simulations
### Parallel Sessions: Thursday, August 3, 2017 (Morning)

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<tr>
<td>11:00A</td>
<td>Rail Negron: A web-based service for distributing curve fitting algorithms onto remote server clusters for improved performance</td>
<td>Hyunsuk Cho: Technology Transition: The Journey from XML to JSON</td>
<td>Benjamin Resnick: The Smart Cities Workshop: Connecting Businesses, Federal Labs, Universities, and Government</td>
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<tr>
<td>11:20A</td>
<td>Annie Bao: Parallelization of Atom-Based Molecular Properties using MPI</td>
<td>Josh Chin: Prognostics and Health Management in Industrial Robot Systems</td>
<td>Anna Liddle: Dance Therapy and Rehabilitative Medicine</td>
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<td>Time</td>
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<td>Lecture Room B</td>
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<tr>
<td>1:30P</td>
<td>Justina Freilich: Analysis of 4D STEM</td>
<td>Benjamin Riley: An Investigation of</td>
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<td>Prompt Gamma Activation and Compton</td>
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<td>and Characterization of Marine Plastics</td>
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<tr>
<td>4:00P</td>
<td>Toyosi Afolabi: Collection and Organization of Adsorption Isotherms for Standard Reference Use</td>
<td>Gregory Fiola: Confirming Calorimetry Metrology - Counting Carbon</td>
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"Certain commercial equipment, instruments, or materials are identified in this paper in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose."
Parks, Samuel - CNST
Saadah, Mariam - CNST
Tatum, Lars - CNST
Torres, Chris - CNST
Whittier, Caleb - CNST
**Title of Talk:** Process Development for Area-Selective Atomic Layer Deposition Using Surface Chemical Patterning

**Abstract:**
Atomic Layer Deposition (ALD) has received significant attention recently for coating the thin films of insulators, semiconductors, and metals with precise control of the film thickness, excellent conformality, and very good uniformity over large areas. However, it remains a challenge to selectively coat a thin film on a defined area by using ALD.

This project is using surface chemical patterning to define the ALD coating area and study the area-selective ALD process on varied substrate materials. Our surface patterning starts with a positively patterned silicon-oxide wafer with photoresist followed by a self-assembled monolayer (SAM) coating and then the photo resist lift off. ALD coating tests are then carried out with or without further chemical surface activation.

By exploring and developing different process conditions, we are improving the film contrast in area-selective ALD coating. We believe that the selectively ALD coating will help people to create devices with permittivity gate oxides, high-k memory capacitor dielectrics, ferroelectric properties, and metals and nitrides for electrodes.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Lars P Tatum
Academic Institution: University of Florida
Grant Number: 70NANB16H
Academic Standing (Sept. ’17): 2nd Year
Future Plans (School/Career): Graduate Studies in Electrical Engineering
NIST Laboratory, Division, and Group: Center for Nanoscale Science and Technology, Electron Physics Group

Title of Talk: Modelling Al nanoparticle localized surface plasmon resonances and the synthesis of Ru-functionalized Al nanoparticles

Abstract:
Electron oscillations are known to occur at the interface of a plasmonic metallic nanoparticle (MNP) when an energy source, e.g. incoming light or high energy electrons, resonates with the free electrons on the metal surface at discrete frequencies. As these resultant oscillations establish standing waves governed by particle geometry, they are known as localized surface plasmon resonances (LSPR). It has been previously shown that surface plasmons may act as a source of “hot” electrons which can promote chemical reactions in a catalytic environment. To better understand such systems at the nanoscale, our group is exploring LSPR phenomena of various MNPs. Here we model aluminum nanoparticle (NP) LSPRs in Matlab using the metal nanoparticle boundary element method (MNPBEM) toolbox. The MNPBEM toolbox simulates a user defined electron beam passing by or through a MNP, estimates LSPRs, and provides the resultant electron energy loss spectroscopy (EELS) dataset. This simulated EEL spectra is then compared with experimental EEL spectra of Al NPs obtained using an environmental transmission electron microscope (ETEM). Concurrently, a synthesis was formulated for decorating plasmonic nanoparticles with a catalyst using a revised incipient wetness impregnation technique. We focused on Al NPs functionalized with ruthenium, a known catalyst. These Ru-functionalized Al NPs were then characterized using the ETEM. The Ru loading was characterized using aberration corrected high resolution TEM imaging, while the chemical composition Ru-functionalized Al nanoparticles was confirmed using EELS. Our results represent practical aspects of exploring and characterizing localized surface plasmon promoted catalytic systems, and is an important step towards understanding plasmonic metals’ contribution to catalytic processes at the nanoscale when excited by an external energy source.

Name: Chris Torres
Academic Institution: University of New Mexico
Grant Number: 70NANB16H
Academic Standing (Sept. ’17): Senior
Future Plans (School/Career): After I graduate from the University of New Mexico, I will go to graduate school to obtain a PhD and pursue a career in academia.
NIST Laboratory, Division, and Group: Center for Nanoscale Science and Technology, Nanofabrication Research Group

Title of Talk: Towards a Scanning Probe Diamond NV Center Nanoscale Magnetometer

Abstract:
The stray fields of magnetic nanostructures can reveal important information about how they function. These structures are found in nanoelectronics, biological cells, chemical reactions, and more. To measure these fields, we are constructing a nanometer-scale tip on the end of a tuning fork cantilever. The scope of this project is to develop a scanning probe instrument to take precise measurements of the surface’s profile, magnetism, and temperature. This project will enable future developments for magnetic measurements near the surface of nanoscale magnets.

The probe will use Nitrogen Vacancy (NV) centers, a type of defect in diamond lattice, to precisely measure temperature and magnetic fields on the nano-scale. In this project, I had to figure out how to hold an NV center defect in an optical microscope’s focal spot, sense surface forces, keep it a fixed distance from the surface, reliably scan the surface, and create an image that tells us about the surface properties. To do this, we decided to explore the non-contact Atomic Force Microscopy (AFM) scanning probe technique due to its non-optical, non-destructive nature. We are constructing this instrument by assembling a quartz tuning fork cantilever on a printed circuit board, then attaching a nanodiamond with NV center to the tip. Throughout the development process, the resonance of the cantilever is monitored closely and characterized due to its importance in AFM.

In our final month, our goal is to perform scanning thermal microscopy of nanostructures as they absorb microwaves at different frequencies. The frequencies where absorption and heating occur offer a precise measurement of the nanomagnets’ properties.

In this talk, I will discuss the design, development, and testing of the scanning probe instrument.
Title of Talk: Development of a High-Etch Resistant Negative-Tone Resist for Electron Beam Lithography

Abstract:
Electron beam lithography (EBL) allows for high-resolution sub-micron patterning of substrates by exposing a layer of resist to a high-energy electron beam, followed by chemical development and subsequent pattern transfer via plasma etching. Commercially available negative- and positive-tone resists such as maN and PMMA can be limiting in their scope, providing high resolution or etch resistance but generally not both. We provide the characterization of a new negative-tone resist with promising resolution and high etch resistance. The resist is spin coated onto silicon and silicon oxide coated wafers and exposed using EBL. After development, the exposed wafers were etched using CF$_4$ and SF$_6$ gas chemistries to transfer the pattern into the substrate. Using a combination of ellipsometry and reflectometry, the etch selectivity of the resist is determined. To confirm feature resolution and aspect ratio, the etched wafers were imaged via atomic force microscopy and scanning electron microscopy. We provide data relating to the resist’s selectivity, resolution, and aspect ratio, as well as a direct comparison between this new negative-tone resist and several well-established positive- and negative-tone resists.
Blanke, Austin - CTL
Galazka, Aneta - CTL
Philp, Chadd - CTL
Shenoy, Vineet - CTL
Name: Aneta Galazka
Grant Number: 70NANB16H

Academic Institution: University of North Georgia
Major: Mathematics

Academic Standing (Sept. '17): Senior
Future Plans (School/Career): Pursue a graduate degree in applied mathematics, subsequently work on independent research and teach

NIST Laboratory, Division, and Group: Communication Technology Laboratory, Wireless Networks Division

NIST Research Advisor: Dr. Fernando Cintrón

Title of Talk: Modeling probabilities for the performance of Device-to-Device communications in the Physical Sidelink Shared Channel (PSSCH)

Abstract: With the prospect of some of the spectrum of Long-Term Evolution (LTE) networks being set aside for public safety users, NIST is developing mathematical models of various control functions for Device-to-Device (D2D) communications, focusing on out-of-coverage scenarios, where User Equipment devices (UEs) are unable to reach a cell tower. D2D wireless devices are used to interconnect and perform three main functions: discovery, synchronization, and communication.

This research models scenarios in the data communication plane, in the Physical Sidelink Shared Channel (PSSCH). It is the next step in studies already completed by NIST modeling overall performance in the LTE network wireless cellular communications rely on a cell tower(s) to allow communication between user's equipment (UEs). In the event of a natural disaster, cell towers can become unavailable, thereby disabling communication between UEs (e.g., smartphones), particularly for first responders. With the newly defined “sidelink” capability for the 3rd Generation Partnership Project (3GPP) Long Term Evolution (LTE) standard, device-to-device (D2D) communications takes the necessity for cell towers out of the equation by allowing first responders' devices to communicate directly with each other. However, LTE D2D communication has limited capabilities, such as: short communication range due to limited power at the UEs, and limits on the number of UEs able to communicate at once due to the distributed nature of the schedule assignment of communication resources in the absence of a cell tower. Enabling frequency hopping for D2D communication will limit the usage of frequency resources experiencing signal degradation due to interference created by other communicating UEs or due to surrounding environment dynamics (e.g., UE mobility, and buildings) that can obstruct wireless signal transmissions or create signal fading. Signal fading can result in either constructive or destructive interference; thus, while some wireless communication channels experience signal attenuation, others could experience a signal amplifying effect. Frequency hopping exploits the signal fading effect by not remaining on the same frequency channel for the entire time duration of a transmission.

The modeling of D2D communications with frequency hopping is crucial to study and determine the configuration settings that will benefit most first responders in line of duty. This project required, (1) to gain deep understanding of LTE D2D communication standard procedures related to frequency hopping; (2) to implement frequency hopping procedure to the NIST LTE D2D modeling platform; (3) to implement test scenarios to validate the module.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Chadd E. Philp
Grant Number: 70NANB16H
Academic Institution: Bowie State University
Major: Computer Science
Academic Standing (Sept. '17): Senior
Future Plans (School/Career): Pursuing a career in Software Engineering
NIST Laboratory, Division, and Group: Communications Technology Laboratory, Wireless Networks Division
Title of Talk: Characterizing User Experience of Voice Application

Abstract:

In 2012, the Congress passed the Middle Class Tax Relief and Job Creation Act of 2012. The act calls for an establishment of a national public safety broadband network to expand high-speed wireless broadband and to improve communications interoperability among first responders. Among communications by first responders, voice is one of the most critical applications. Voice quality is crucial in a first responder’s line of work, and it could be a matter of life and death. Focusing on voice quality, this project is to investigate and implement mechanisms to translate network performance metrics, e.g. packet loss rate and delay, into quantifiable user experience levels.

Network operators have various methods and categories available to achieve a proper voice quality assessment. Specifically, there are the subjective versus objective methods and the listening-opinion versus conversation-opinion categories. Based on the goals for this project, the objective method that provides the conversation-opinion scores is desired, and this leads to the E-model (ITU-T G.107) to serve as a base for the research. The E-model is a common tool for assessing the combined effects of variations in transmission parameters that affect the conversational quality. The fundamental principle is that the psychological and physical system factors are additive and the primary output produced is called the R-factor, which is a scalar rating of the transmission quality.

Using the E-model, we developed a Python program to test different scenarios to illustrate the change in R-factor over the length of the transmission. The outcomes of the project are planned to be used as inputs into network control algorithms, such as admission control and preemption algorithms, with the goal of maximizing the amount of traffic the public safety network could serve, while ensuring that first responders receive services at the required level of quality.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Vineet R. Shenoy
Grant Number: 70NANB16H
Academic Institution: Rutgers University
Major: Electrical Engineering, Computer Science
Academic Standing (Sept. '17): Senior
Future Plans (School/Career): Pursuing a PhD in Electrical Engineering
NIST Laboratory, Division, and Group: Communications Technology Laboratory, Wireless Networks Division
NIST Research Advisor: Dr. Anirudha Sahoo
Title of Talk: Simulation of SAS-CBSD protocol for the CBRS band

Abstract:

As the number of wirelessly-connected devices increases, the electromagnetic radio spectrum, over which devices communicate, becomes scarce and congested. The scarcity is further exacerbated due to exclusive licenses granted by the Federal Communication Commission (FCC) and severe under-utilization of spectrum by the licensees. To address these issues, the FCC has opened up 150 MHz in the 3.5 GHz band, called the Citizens Broadband Radio Service (CBRS) band, for commercial use on a priority based sharing. A Spectrum Access System (SAS) will be responsible for managing the commercial CBRS Devices (CBSDs) such that the CBRS rules set by the FCC are adhered to by the CBSDs during operation.

The Wireless Innovation Forum (WinnForum) has developed a specification for the protocol to be run between a SAS and a CBSD. In this project, we develop a simulator for the SAS-CBSD protocol using Omnet++. The simulator will model the requests from the CBSDs and responses from the SAS and implement the state machines published in the WinnForum specification. The protocol has few configurable parameters which are left open to the implementers. The simulator will be used to study the impact of these configuration parameters on the performance of the protocol. The simulator will also be helpful in studying the protocol under various stress conditions.

A robust simulator will provide insights into various configurations of CBRS deployment. It will also provide details regarding the strengths, weaknesses, and limitations of current protocols which will be helpful to the industry as well as to the regulatory bodies.
Aboul-Enein, Omar - EL
Antia, Rushad - EL
Bichenevicius, Michael - EL
Burns, Christian - EL
Burtwistle, Charles - EL
Chien, Jeffrey - EL
Chin, Joshua - EL
Chinn, Edward - EL
Chordia, Shivang - EL
Chun, Hyunsoo - EL
Crockett, Emma - EL
de Oliveria, Samuel - EL
Fangmeyer, Ryan - EL
Farzana, Fateema - EL
Fernandez, Joshua - EL
Fiola, Gregory - EL
Garner, Jonathan - EL
Gibbons, Nathaniel - EL
Gonzalez Perez, Massiel - EL
Henderson, Bradley - EL
Hodgkinson, David - EL
Idrogo, Nathan - EL
Lacey, Thomas - EL
Lai, Trinh - EL
Larson, Eric - EL
Liu, Julie - EL
Ludwig, Sierra - EL
McIntyre, Rachel - EL
Mennu, Matlock - EL
Mullin-Conant, Ashby - EL
Nicholson, Elias - EL
Nukuro, Dilnesa - EL
Pickett, Jacob - EL
Piland, Jonathan - EL
Rafizadeh, Ramin - EL
Salpietro, Vincent - EL
Schovanec, Cory - EL
Serrano Ragsdale, Nicolas - EL
Shan, Bohan - EL
Smith, Stephan - EL
Smith, Weston - EL
Spector, Samuel - EL
Thomas, Austin - EL
Winnard, Thomas - EL
SURF Student Colloquium
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Name: Omar Aloul-Enein
Grant Number: 70NANB17H105
Academic Institution: Salisbury University
Major: Computer Science and Mathematics

Academic Standing (Sept. ’17): Senior
Future Plans (School/Career): Going forward, I will pursue graduate studies in computer science, and I am currently researching graduate programs within the state of Maryland. In addition, I will continue to apply for opportunities at NIST while pursuing a career in research.

NIST Laboratory, Division, and Group: Engineering Laboratory, Intelligent Systems Division, Mobility and Manipulation Systems Group
NIST Research Advisor: Roger Bostelman
Title of Talk: Performance Measurement of Mobile Manipulators: Expansion to Autonomous-Unmanned Ground Vehicles (A-UGVs)

Abstract:
For the past three years, the Robotic Systems for Smart Manufacturing (RSSM) Program has sought to understand the performance of a specific class of robots known as “mobile manipulators”. Within industry, these robots hold the potential to offer a more flexible, dynamic workflow since a manipulator, which is normally constrained to a single workspace, can now perform multiple assembly tasks across several, distinct locations. However, the integration of mobile manipulators within today’s manufacturing systems often requires an expensive and time consuming calibration process. Furthermore, leveraging their ability to adapt to multiple workspaces requires an acute understanding of the problem posed by coordinate registration to the workspace. To ease this burden and foster a wider understanding of the performance uncertainty characterizing these systems, the RSSM Program has focused on development of an accessible and cost-effective artifact-based performance measurement concept for both mobile manipulators and their corresponding registration methods. The uncertainty of the measurement concept is compared to a ground-truth defined by measurements taken with an optical tracking system (OTS). While previous developments have seen testing of the existing methodology on a mobile manipulator consisting of an Automatic – Unmanned Ground Vehicle (as termed within ASTM F45), there is still a need to support the utility of the concept when applied to various mobile manipulator systems and registration technologies. Therefore, the work completed this summer focused on expanding the implementation of the existing measurement concept to a separate mobile manipulator system utilizing an Autonomous - Unmanned Ground Vehicle. The vehicle of this system uses navigation technologies not present in the vehicle of the existing implementation including an onboard laser for simultaneous localization and mapping (SLAM). New developments included the implementation of inter-system communications between the two mobile manipulator robots and adaptation of existing code bases for laser spiral search localization and bisection registration of reflectors mounted to the artifact. In addition, comparison of the new implementation against OTS was conducted.

Name: Rushad Antia
Grant Number: 70NANB17H164
Academic Institution: University of Maryland
Major: Computer Science

Academic Standing (Sept. ’17): Sophomore
Future Plans (School/Career): Finishing school & finding a future in app/game development

NIST Laboratory, Division, and Group: Engineering Lab, Intelligent Systems Division, Network Control Systems
NIST Research Advisor: Richard CanedeII, Mohamed Haney
Title of Talk: We Found Wireless in a Wired Place

Abstract:
The Industrial Wireless Project is conducting cyber-physical systems research aimed at measuring the performance of various physical systems when fit with wireless communication technologies. The current factory setting utilizes wired communications for sensing and actuation; however, it cannot sustain because of the high costs of installation and upkeep. This project’s goal is to measure how reliable wireless communication (802.11 b/g/n) works in a factory setting.

To do this, we developed a Publish/Subscribe Network library in Node.js to run on Intel® Edison Development boards so that we could build a distributed intelligence system. This system allows multiple nodes to publish their state to other nodes that subscribe to said state. Given this information, they connect to a “Master Node” which automatically brokers connections between the nodes. Along with the network package, we also developed a website that allows the user to remotely monitor and interact with all the devices. This type of system enables us to see the performance and reliability of a wireless system when brought into a factory setting.

After the development of the network package, we plan to connect each device to a Radio Frequency Channel Emulator (RFCE) where we can simulate a factory setting and perform various tests to measure latency, jitter, and throughput. Ultimately, we would like to see how badly Wi-Fi performs in an industrial setting.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Michael Bichnevicius
Grant Number: 70NANB17H089
Academic Institution: The Pennsylvania State University
Major: Mechanical Engineering

Future Plans (School/Career): Attend graduate school
NIST Laboratory, Division, and Group: Engineering Laboratory, Energy and Environment Division, Heating Ventilation Air Conditioning & Refrigeration (HVAC&R) Equipment Performance Group
NIST Research Advisor: Harrison Skye
Title of Talk: Testing Low Global Warming Potential Refrigerants

Abstract:
Refrigerants are the working fluids in heating, air-conditioning, and refrigeration systems. Following the adoption of an amendment to the Montreal Protocol in 2016, most hydrofluorocarbon (HFC) refrigerants currently in use will be phased out or phased down due to their high global warming potentials (GWPs). Consequently, candidate replacement fluids must be researched and evaluated; candidates must have a very low GWP in addition to zero ozone depletion potential (ODP), low flammability and toxicity, and thermodynamic properties compatible with current equipment.

Hydrofluoroolefins (HFOs) are a promising set of chemicals with exceptionally low GWP and zero ODP. The overall GWP impact of refrigerants is caused directly by fluid released into the atmosphere and indirectly by emissions from the power plant generating electricity for the associated HVAC&R equipment. Because the indirect emissions contribute far more to the overall GWP impact, it is essential that the efficiency of each replacement refrigerant is quantified to help find fluids that achieve a net reduction in total GWP impact. R-1234yf and R-452B are two HFOs that have been introduced to replace R-134a and R-410A respectively. R-134a is used in refrigerators and automobile air conditioners, while R-410A is used in residential and light commercial air conditioning systems.

A heat pump test apparatus was used to measure the cycle performance of R-1234yf and R-452B. The temperatures, pressures, and mass flow rates of each refrigerant and the heat transfer fluids were used to calculate the coefficient of performance (COP) and volumetric capacity at multiple Air Conditioning, Heating, and Refrigeration Institute (AHRI) standard rating test conditions. Several vapor-compression cycle configurations were tested by varying the number of tubes used in the evaporator and condenser, including or bypassing a liquid-line/fusion-line heat exchanger, and targeting multiple capacities. The results will be compared to data taken previously on this apparatus for R-134a and R-410A. In addition, the measurements will be used to verify a NIST heat pump modeling tool, CYCLE_D-HX, which can be used to explore other fluids.

Christian J. Burns
Grant Number: 70NANB17H106
Academic Institution: Shepherd University
Major: Computer Engineering

Future Plans (School/Career): Pursuing a career in industrial control systems and automation while also attending graduate school
NIST Laboratory, Division, and Group: Engineering Laboratory, Intelligent Systems Division, Network Control Systems Group
NIST Research Advisor: Timothy Zimmerman
Title of Talk: Impacts of Cybersecurity on Industrial Robotic Systems

Abstract:
The next trend in manufacturing is for information to become more easily accessible. Many industrial control systems (ICS) are being connected to the internet or other large networks. Connecting manufacturing systems to large networks has both positive and negative implications related to the overall productivity of a factory. The positive aspect of bridging communication gaps of these systems is that data is easier to access and manage, which ultimately can yield to a significant rise in overall factory efficiency. In regards to the negative side of connectivity, these avenues for data now must be protected from cyberattacks. Implementing cybersecurity to counter these potential threats can alter the timing and reliability of ICS communications which could create uncertainty in factory performance.

This project examines the impact of cybersecurity tools (firewalls, antivirus, etc.) on industrial control systems. The first objective within this project is to create an environment for this research to resemble other ICS networks in the real-world. To achieve this, we developed software to simulate manufacturing work cells. These work cells are loaded on single-board computers which are installed within the robotic enclave. The research will examine the effects of network variables within multiple locations of the ICS network. Through this research, we will be able to determine the best practices for cybersecurity.
**Title of Talk:** Measuring the Economic Value Of Resilience Investment

**Abstract:**
A Computable General Equilibrium (CGE) model is used to model economic interactions and analyze the impact a change would have on a community. They can help decision-makers by showing how an economy would react to a disaster, policy change, or other “shocks”. These models are large-scale, non-linear, optimization problems far too complicated to solve by hand and must be solved computationally using software. This can be done using an algebraic modeling language (AML). The purpose of an AML is to allow the programmer to code in a syntax very similar to the mathematical notation of the problem. While several well-established commercial AMLs exist, such as GAMS or AMPL, they are far from cheap to use. The goal of this project was to create an open source, object-oriented, CGE. This was done by porting existing GAMS code to python using the pyomo package, which allows the programmer to use python as an AML. Another advantage of an AML is that writing the problem is independent of the solution method. Having an open source, object-oriented program like this easily allows a user to create complex models and update them without having to re-write code to solve them. Once these models are created, a user can repeatedly load different data and solve them to analyze changes. This code will form the basis of using CGE models to quantify the economic value of investing in disaster resilience. Investing in resilience, while important, is neither simple nor inexpensive. Thus, being able to analyze how it will affect an economy is crucial. Seeing the economic value of resilience investments will help decision-makers examine the advantages in preparing for, rather than reacting to, disasters.
**Title of Talk:** Prognostics and Health Management in Industrial Robot Systems

**Abstract:**

Prognostics and Health Management (PHM) is the discipline that focuses on monitoring, diagnostic, and prognostic techniques to enhance maintenance strategies. PHM has helped guide the development of the predictive maintenance strategy; actively monitors the health of equipment and predicts the remaining useful life of that equipment. If effectively deployed, predictive maintenance can lower both planned and unplanned downtime thereby increasing process productivity. NIST's Prognostics, Health Management, and Control project is performing research to develop test methods, reference data sets and algorithms to be used by manufacturers to design and implement PHM within their own manufacturing processes.

There are many criteria that can be used to evaluate the health of an industrial robot system. One specific research focus is on robot accuracy to support overall robot system health assessments. Several test methods are developed that could be used to assess robot accuracy over time. To effectively monitor robot accuracy, robot arm failures must be isolated from failures of other components such as part, gripper, or fixture failures. Additional methods are developed to distinguish between these types of failures. A key component of these test methods is the use of test artifacts. Test artifacts are physical objects that the robot interacts with to obtain data related to robot health. To collect this data, a 6-axis force and torque sensor is mounted between the robot's tool flange and end-effector, and is used to detect forces created by contact between the test artifacts and the robot's end-effector.

Early results indicate that robot joint degradation can be effectively monitored by testing robot accuracy in each Cartesian degree of freedom, individually. Additionally, these methods have shown that robot failures can be isolated from other types of failure.

**Title of Talk:** Colorimetric and Spectroscopic Analysis of Automotive Paint Samples

**Abstract:**

Trace evidence is a small piece of evidence left at a crime scene which can be used to identify or link a person with a crime. An example is car paint which is left behind in car accidents. This trace evidence can be used to classify the car of the perpetrator. Previously, much of the analysis of trace paint specimens was done qualitatively by comparison with standard reference samples via the naked eye. The overall goal of the project is to develop a quantitative method of analyzing and matching a car paint sample with the car's make, model, and year. The immediate goals of this project are determining the level of uncertainty in trace paint measurements between different Fourier Transform Infrared (FTIR) spectrometers via an interlaboratory study and assessing the use of handheld spectrophotometers, which differ in aperture size and configuration geometry, to determine quantitative color measurements. It is expected that the uncertainty in IR spectra can be determined and that the handheld spectrophotometers can be used interchangeably.

The FTIR interlaboratory study consisted of analyzing the two paint specimen consisting of four different layers of automotive paint on five different FTIR spectrometers. The uncertainty in the measurements will be determined by ratioing intensities of characteristic peaks in the FTIR spectra. The FTIR peaks are chosen based on the chemical structure of the polymer used in automotive paint. The method for assessing the handheld spectrophotometers is the use of test artifacts. Test artifacts are physical objects that the robot interacts with to obtain data related to robot health. To collect this data, a 6-axis force and torque sensor is mounted between the robot's tool flange and end-effector, and is used to detect forces created by contact between the test artifacts and the robot's end-effector.

Early results indicate that robot joint degradation can be effectively monitored by testing robot accuracy in each Cartesian degree of freedom, individually. Additionally, these methods have shown that robot failures can be isolated from other types of failure.
Additive manufacturing (AM) is the process of building an object up by adding layers of material on top of one another. The data generated pre, during, and post build is essential to improving AM technologies. Data from thousands of builds can be stored and analyzed to give a better understanding of the process and its outcomes – however, there needs to be a database that properly stores, displays, queries and manages this data. A working AM database that is populated with comprehensive data, straightforward to use, and accessible to the public is lacking, but currently in the works as NIST’s Additive Manufacturing Materials Database (AMMD). This ever-growing database will include packages to analyze data, so that correct decisions regarding AM can be made.

When preparing a build using the AM process, there are many different variables that can be recorded – material, grain size, grain direction, etc. AMMD data can be stored on local or cloud servers through the use of MongoDB, and analysis of this data can then be conducted using several different programs – Python, Matlab, and R. However, NIST has not provided methods or guidelines to properly query and analyze AMMD data, it was essential to create open-source scripts that could do exactly that.

In support of AMMD efforts, data created by several institutions including NIST was manually uploaded into a local AMMD database.

Different packages of code were created with the ability to interact with the server, pull data, query, and sort it accordingly. A key feature of creating open-source scripts is the ease of use; as they may have a purpose in many different formats. Creating robust code with clear comments that can be used in different formats is essential to supporting diverse groups of AM analysts. Creating a database and query system that supports uniformity throughout industry helps to standardize the core fundamentals of data acquisition, storage, and analysis for additive manufacturing.

For nearly 20 years Extensible Markup Language (XML) has been the mainstream syntax used for data exchange supported by its XML Schema counterpart. In recent years, as browser-based applications, which rely heavily on JavaScript language become more popular due to the increasing uses of mobile applications and cloud computing, JavaScript Object Notation (JSON) has gained momentum as another syntax for data exchange. For standard organizations and companies that have invested in information technologies based on XML, the emergence of JSON requires a lot of planning and considerations. In this presentation, we will present industry requirements and factors needed to be considered for JSON adoption in the data exchanges for mobile applications integration. We will then summarize the work we have done over the two-month period to assist manufacturing companies that rely on data exchange standards to run their daily-productions and other business transactions.
Name: Emma Crockett
Grant Number: 70NANB17H074
Academic Institution: The George Washington University
Major: Electrical Engineering
Academic Standing (Sept. '17): Senior
Future Plans (School/Career): Attending a 5th year at the George Washington University to earn a graduate degree.
NIST Laboratory, Division, and Group: Engineering Laboratory, Energy and Environment Division, Heat Transfer and Alternative Energy Systems Group
NIST Research Advisor: Behrang Hamadani
Title of Talk: Energy Scavenging for Low Power Applications Using Ambient Indoor Light

Abstract:
Energy is one of the main limitations as the concept of the Internet of Things becomes more prevalent. The vision of large interconnected networks of wireless sensors is accompanied by the nightmare of constant battery replacement and disposal. Our hope is that systems can self-scavenge limited energy from ambient heat, light, radio, or vibrations from the surrounding environment. This research focuses on energy scavenging of ambient indoor light to power sensors or other small-scale, low-power electronics.

During this project, we looked at several different types of solar cell technologies to determine which technologies most efficiently extract energy in low light conditions. We tested each of these technologies under various spectra of light to determine which solar cells function most efficiently under various levels of luminous flux of white light, warm light, and cool light. To charge rechargeable lithium-ion batteries in a safe and practical way, we built a smart charger unit by reconditioning a USB charging circuit for solar charging. The smart charger was also designed to monitor and measure the supplied input current and voltages and the output charging current and voltages simultaneously. A LabVIEW program was written to monitor these measured quantities. We also designed custom PCB for building photovoltaic minimodules suitable for our indoor light harvesting needs.

The results of these experiments showed that energy harvesting from ambient indoor light is a possible and practical way to power the Internet of Things. Networks of wireless sensors can be powered by the environment they are placed in by recycling ambient light into energy that can be stored in a small, rechargeable lithium-ion battery. Additionally, the color spectrum tests showed that the efficiency of solar cell technologies is dependent on the color spectrum of the light they are present in.
**Name:** Ryan Fangmeyer  
**Grant Number:** 70NANB17H087  
**Academic Institution:** North Carolina State University  
**Major:** Mechanical Engineering  
**Academic Standing (Sept. '17):** Junior  
**Future Plans (School/Career):** Complete my B.S in Mechanical Engineering and pursue a master's degree in Engineering  
**NIST Laboratory, Division, and Group:** Engineering Laboratory, Systems Integration Division, Information Modeling and Testing Group  
**NIST Research Advisor:** Yan Lu  
**Title of Talk:** Additive Manufacturing Material Database Schema  

**Abstract:**  
Additive Manufacturing (AM) uses digital models of geometry to drive the deposition of materials layer by layer to build a three-dimensional object. As the AM industry grows, there has been inadequate supporting technology and data to support process repeatability, a major barrier in adopting AM as a production technology. In response, An Additive Manufacturing Material Database (AMMD) is under development by NIST, which has the ability to store comprehensive data from AM builds and identify relationships between pre-build processes and material structure.  

AMMD data is formatted using an eXtensible Markup Language (XML) Schema, and displayed with a customizable web graphic user interface and ontology. The Schema has been designed to incorporate the overarching life cycle of the AM material and builds, from feedstock material to post-build. The process behind building the Schema is on-going, and requires research and tests to be conducted in order to determine what should be included in the Schema design. Research on AM testing was conducted to determine a standard format for certain facets of the Schema, including microstructure, tensile, thermal, and chemical properties of AM builds. Each of the supporting data files and interfaces were brought in-line with the Schema, including an ontology to support visualization. A tool based on Extensible Stylesheet Language Transformations (XSLT) was developed and used to translate legacy .xml data files to updated Schema formats. As new data sets and Schemas are implemented, there are growing possibilities to establish correlations between processes, materials, and builds.
**SURF Student Colloquium**  
**NIST – Gaithersburg, MD**  
**August 1-3, 2017**

**Name:** Joshua Fernandez  
**Grant Number:** 70NANB17H124  
**Academic Institution:** University of Maryland, Baltimore County  
**Major:** Mechanical Engineering  
**Academic Standing:** Junior  
**Future Plans:** Graduate School  
**NIST Laboratory, Division, and Group:** Engineering Laboratory, Materials and Structural Systems Division, Community Resilience Group  
**NIST Research Advisor:** Ken Harrison  
**Title of Talk:** Lumberton Flood Resilience Decision Support Tool

**Abstract:**

The goal of community resilience planning is to enable communities to be able to recover quickly from natural or man-made hazard events so that people can resettle and return to their normal lives. The Community Resilience Group is tasked with helping this objective become a reality in every community across the nation. By researching and creating code standards, establishing local collaborative planning teams, and investigating disasters, they take steps toward building safe and secure communities. One specific tragedy that the Community Resilience Group investigated was the flooding in Lumberton, North Carolina due to Hurricane Matthew in October 2016. This event caused several injuries and deaths, as well as inundating integral systems within Lumberton. In addition, the entire population in the floodplain was forced to temporarily leave their homes until the community could be repaired. Projects are currently underway at NIST to help prevent similar disasters from happening again. This talk will focus on my development of a simplified model to support resilience planning for communities such as Lumberton that are subject to flooding hazards. Looking at a range of flood stages, the model calculates estimates of restoration cost and repair time of homes and other systems within Lumberton. The model also allows users to input mitigation techniques that reduce flood damage and allows users to see their consequences. By using the model as an investigative tool, we can anticipate how flood-preventive action (or inaction) impacts the community. With the results of the model in mind, we will be able to make more informed decisions that can help protect many communities from the disasters of flooding.

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**Name:** Gregory Fiola  
**Grant Number:** 70NANB17H164  
**Academic Institution:** University of Maryland, College Park  
**Major:** Fire Protection Engineering  
**Academic Standing:** Senior  
**Future Plans:** Continue Fire Research in graduate school  
**NIST Laboratory, Division, and Group:** Engineering Laboratory, Fire Research Division, National Fire Research Laboratory  
**NIST Research Advisor:** Rodney Bryant  
**Title of Talk:** Confirming Calorimetry Metrology - Counting Carbon

**Abstract:**

The National Fire Research Laboratory (NFRL) houses an array of exhaust hoods that have the capability of accurately measuring heat release rate from combustion experiments using the principle of oxygen-consumption calorimetry. In addition to heat release rate, the NFRL gathers further measurements that can be used for quality control. Large scale burners act as precision sources of heat, where natural gas serves as a fuel that is readily available in large quantities, and most importantly, well characterized. Careful measurement of the flow and composition of natural gas allows for accurate calculations of predicted heat energy release, which is used to confirm independent heat release measurements directly from the exhaust gas calorimetry system. While this method is well established and proven, it does not allow for easy explanation of outliers and variation without isolation of derived parts. Thus, deploying the law of conservation of mass, another predicted vs. direct experiment can be balanced by cross-validating the flow of carbon dioxide into and out of the calorimetry system. This carbon balance supplements the evaluation of the energy balance by using fewer variables and assumptions, resulting in stronger confirmation and reduced uncertainty. With both an energy balance and carbon balance, uncertainty analysis can be better used to investigate sources of measurement bias and begin further research in reducing uncertainty contributions of individual variables and assumptions. Each measurement method, predicted and direct, was reported with an estimated expanded uncertainty of ±2% and ±4%, respectively, and cross-validated with a cumulative average relative difference of about 1%. Results and methodology of this research are expected to improve fire metrology, where better heat release rate measurements allow for better flammability characterizations of products and materials, improved codes and standards, and a world safer from the threat of fire.
**Title of Talk:** Advanced Sensing Development to Support Robot System Prognostic and Health Management (PHM)

**Abstract:**

The accuracy of a robotic arm determines its ability to function precisely and effectively, especially in a manufacturing environment. Over time, a robot's calibration and performance degrade which can cause unexpected shutdowns, costing manufacturers significant time and money. Thus, manufacturers face the challenge of maintaining robot performance and developing maintenance strategies to preserve production efficiency. The goal of the Prognostics, Health Management, and Control (PHMC) project is to develop the necessary measurement science to support the monitoring, diagnostics, and prognostics of robot accuracy degradation. In project research includes modeling for the test method, an advanced 7-Dimension (time, X, Y, Z, roll, pitch, and yaw) perception sensor to measure a robot's movement, and algorithm development to analyze the subsequent data.

To track the 7-D perception sensor, a stereo camera system is used to test the robot accuracy. A sensor identification and tracking algorithm was developed in MATLAB to determine the exact center line of the sensor with sub-pixel accuracy. The algorithm uses image filters and differences in light intensity between the sensor and the background to determine the location of the sensor and its center. In the future, the sensor will have the capability of changing color and thus other methods may be used for more accurate and efficient identification. A graphical user interface (GUI) was created to implement the camera's software development kit (SDK) to control the camera and the identification algorithm written in MATLAB. The MATLAB algorithm was rewritten in C++ to work with the GUI and to process the high-speed stream of images from the two cameras. As the 7-D sensor reaches a final design, the sensor identification algorithms will be calibrated and modified to function with the final sensor. In the future, the algorithms will be used to track the sensor and extract data to determine the health of the robot and its accuracy, alerting manufacturers before a robot breaks down and preventing losses in productivity.
Disaster literature covers a vast research on different areas of recovery but the household recovery topic is still not clear. Understanding household recovery and its different components provides the foundation for more efficient models, recovery tools and policies that contribute to a more resilient community. The goal of disaster research is to provide information that supports better mitigation, disaster preparedness, response, and recovery of all groups that make a community whole. This review focuses on the household as any group of people sharing the same house; its recovery requires improvements to the housing, physiological stability, and economic recovery. A literature review was conducted to identify different definitions of household recovery across the preexisting recovery research. Various combinations of Boolean operators and keywords were generated to pull results from two different electronic databases. Articles were screened for their ability to address specific research questions on household recovery definitions, measurement, stages of recovery, and causal factors affecting recovery. Researchers seldom describe household recovery and its webbed components; instead, they interchangeably use the terms housing and household as the same. The measurement of household recovery is often focused on one of its dimensions: housing (physical structure), economic, or physiological. No study was found on a complete multidimensional measurement of household recovery. This research extended into the physical and mental health recovery of the household since many studies describe this as an important component, but do not address the link between housing recovery and the health recovery of its residents. The results of this review stress the link between the components that make up household recovery. For the household to completely recover, the housing/shelter structure and lifelines must be recovered, its members must reach some level of mental and physical recovery, and have access to their income sources, schools and other social connections.
### David Hoddinott

**Grant Number:** 70NANB17H092  
**Academic Institution:** Rensselaer Polytechnic Institute  
**Major:** Aeronautical engineering  
**Academic Standing** (Sept. '17): Sophomore  
**Future Plans (School/Career):** Graduate school in Aerospace or mechanical engineering  
**NIST Laboratory, Division, and Group:** Engineering Laboratory, Fire Research Division, Flammability Reduction Group  
**NIST Research Advisor:** Morgan Bruns  
**Title of Talk:** Analysis of vegetative fuels for wildfire modeling

**Abstract:**  
The ability to accurately predict how a potential wildfire will burn and spread is essential when designing safe buildings and infrastructure, particularly in areas where wildlands meet urban areas. Throughout the last decade, the accuracy of these predictions has been greatly improved by computational fire models such as NIST’s Fire Dynamics Simulator (FDS). A key input to modeling behavior of a wildfire with FDS is the type of fuel that the wildfire consumes. Having a more accurate understanding of how different species of vegetation burn, combined with knowledge of where that vegetation is found will improve the accuracy of fire modeling, therefore advancing our ability to predict and protect against wildfires. Several different species of plants were sampled repeatedly between May and August of 2017 to observe differences between species, as well as how newer foliage compares to more established foliage. Thermogravimetric Analysis (TGA) is a method of thermal analysis in which the mass of a sample is measured as a function of temperature or time to infer physical or chemical changes the sample undergoes as it’s heated. By running TGA tests on the vegetation samples we can learn when reactions occur and the fraction of the sample that decomposed as a result of each reaction. Kinetic parameters can be calculated from this data, which in turn can be used as inputs to FDS, resulting simulations that are more representative of actual wildland fires.

### Nathan Idrogo

**Grant Number:** 70NANB17H115  
**Academic Institution:** Texas Tech University  
**Major:** Civil engineering  
**Academic Standing** (Sept. '17): 1st year graduate student  
**Future Plans (School/Career):** Pursue a Master’s degree at Purdue University, gain experience in industry, and eventually earn a PhD in civil engineering  
**NIST Laboratory, Division, and Group:** Engineering Laboratory, Materials & Structural Systems Division (MSSD), Disasters and Failures Studies Group  
**NIST Research Advisor:** Judith Mitrani-Reiser  
**Title of Talk:** Best Practices in Sampling Methods for Post-Disaster Investigations

**Abstract:**  
Natural hazards are a significant threat to the well-being of millions of Americans and to the progress of our nation. For more than 40 years, NIST has played a major role in conducting investigations and providing recommendations after such hazards become disasters, such as in the case of Hurricane Katrina in 2004 or the May 22, 2011 Joplin, Missouri tornado. The focus of investigating disasters and structural failures was formalized into a new program at NIST: Disaster and Failures Studies (DFS) program. In large-scale disasters, challenges arise in statistically assessing building performance across affected communities in a representative way. Traditionally, disasters are investigated through ground surveys, where scientists, engineers, and other officials survey facilities and associated stakeholders. Ground surveys can be inefficient but are accurate and detailed. On the other hand, emerging technology offers ways to quickly and representatively survey large areas, but with less accuracy. Traditional and newer tools have their respective strengths and weaknesses, but deciding which methods or a combination of methods is most appropriate is important for an impactful investigation. However, DFS has not historically used standardized sampling protocols for research studies and investigations. Therefore, it is necessary to perform a literary review of disaster investigations, representative sampling methods, and technology that have been used to evaluate building and infrastructure performance, as well as technical aspects of evacuation and emergency response procedures that contributed to injuries and fatalities during the event. This summer project will conclude with a toolbox of effective and reliable sampling methods and tools that can be incorporated into the DFS deployment decision-making algorithm. The development of best practices in sampling methods is expected to address the inherent challenges of data collection for large populations, ensure that the DFS is updated about the most recent reconnaissance technology available, and initiate the standardization of a sampling methodology.
**Abstract:**

Graphene oxide (GO) nanofillers can enhance the strength, thermal stability, and barrier properties (i.e., corrosion resistance) of polymer coatings. Graphene oxide (GO) is also considered an ideal nanofiller candidate for polymer nanocomposites (PNCs) due to its low cost and ease of processing. In the case of typical polymer materials, weathering conditions such as ultraviolet (UV) radiation, heat, and moisture can lead to degradation. This process is also expected to occur for GO/PNC coatings, but the impact of GO on polymer degradation is unknown. For this reason, the effect of GO on the durability of polymer coatings was investigated to assess material service life. The exposure of GO during the degradation process was also monitored to evaluate environmental, health, and safety issues.

For this study, two different GO loadings, 0.4% w/w and 1.2% w/w, were dispersed into waterborne polyurethane (WBPU) and characterized. The unfilled WBPU controls and the GO/WBPU nanocomposites were then exposed to different weathering conditions using the NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure), an accelerated weathering device with independent temperature and humidity controls that uniformly irradiates samples with high-intensity UV light (140 W/m² at wavelengths from 295 nm to 400 nm). UV-exposure of the samples was performed under dry and humid conditions, both at a high temperature (55 °C) to accelerate weathering. Samples were also weathered under the same conditions without UV light. Various techniques were used to characterize GO/WBPU nanocomposites as a function of GO mass loading to measure the weathering transformations of GO/WBPU nanocomposites relative to unfilled WBPU controls. The techniques used in this study included attenuated total reflection - Fourier transform infrared spectroscopy (ATR-FTIR), Raman spectroscopy, scanning electron microscopy (SEM), and mass loss after weathering. Data was collected at several different exposure times of accelerated weathering.
**Title of Talk:** ATR-FTIR Analysis of Different Backsheet Compositions

**Abstract:**
Backsheets provide environmental and electrical isolation, functioning as a mechanical barrier, and a method of diffusion control for photovoltaic cells. Real world weathering stressors such as light and temperature play a critical role in the degradation of backsheets. Such degradation can compromise the isolation of the cell resulting in power loss or failure of the module. Long exposure times, module cost, and varying environmental conditions for field modules frequently require researchers to adopt artificial weathering techniques for the analysis of photovoltaic modules and their components. The standardization of such techniques is essential to obtain reliable results; thus, the International Electrotechnical Commission has adopted standard conditions for the weathering of photovoltaic components.

Fifty-six backsheet samples, representative of the current and future photovoltaic backsheet market, were exposed under the proposed IEC TS 62788-7-2 guidelines. The evaluation of such materials under standardized weathering conditions is critical to the selection of backsheets and the development of the photovoltaic technology. The present work is in collaboration with NREL where mechanical testing was performed on the backsheets. An ATR-FTIR procedure was developed to characterize the different backsheets, relate the chemical properties with the mechanical found at NREL, and to provide chemical explanations for physical deformities, including cracks.

In comparing UV exposed and thermal exposed PVF backsheets, it was found that the UV exposed backsheets underwent an increase in oxidation with increasing exposure time. Acrylate PVDF showed a decrease in the polyester group after UV-exposure; while, PET showed a transition in the carbonyl region and the formation of carboxylic acid. Upon thermal exposure EVA showed an increase in oxidation possibly resulting in the cracks found in the mechanical testing at NREL for the heat exposed side of EVA. Finally, all transparent backsheets that have potential use for the new bifacial PV modules were degraded substantially in both the exposed and unexposed sides of the backsheets indicating that caution is needed when selecting a backsheet material for this new technology.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Sierra Ludwig
Grant Number: 70NANB17H131
Academic Institution: Boise State University
Major: Mechanical Engineering

Academic Standing (Sept. '17):
Senior
Future Plans (School/Career):
Graduate in December and work in industry for a few years before pursuing a master’s degree in ergonomics
NIST Laboratory, Division, and Group:
Engineering Lab, Materials and Structural Systems Division, Structures Group
NIST Research Advisor:
Travis Thonstad, Jonathan Weigand, & Joseph Main
Title of Talk:
Condition Assessment of Concrete Infrastructure using Photonic Sensor Networks

Abstract:
Bridges, dams, tunnels and nuclear facilities are just a few examples of infrastructure that keeps America connected, they are also examples of infrastructure that is literally falling apart as a result of being used well past the intended service life. Over time these concrete structures start to degrade from the inside out, but sub-surface assessments using nondestructive testing are typically only carried out once degradation is visible. Real-time, distributed sensing technologies are not yet in widespread use, in large part because the capability of these systems to detect widespread infrastructure deterioration has not been demonstrated. Past research has shown that photonic sensors, such as Fiber Bragg Gratings (FBGs) etched into optical fibers, can be used to reliably measure strain when embedded in concrete structures. This research involves evaluating the viability of an embedded network of photonic sensors for condition assessment of concrete infrastructure. Such sensor networks would be used to measure accumulated strains under service load and could also detect the formation of defects through measurement of ultrasonic wave propagation through the structure. To test the feasibility of such sensor networks, two 15.24 cm x 30.54 cm (6 in x 12 in) concrete cylinders were cast, each with an array of four embedded FBG sensors. The viability of externally applying FBG sensors for measurements on existing structures was also investigated using multiple techniques. A third specimen incorporated embedded FBG sensors for measurement of temperature and relative humidity. Temperature measurements enable temperature compensation of measured strains, while humidity measurements enable detection of water ingress, which leads to corrosion of reinforcing steel.

To evaluate the sensor networks, the concrete cylinders were tested under both monotonic compressive loads and ultrasonic excitation. Changes in temperature and humidity associated with curing of the concrete were also measured. The results of these pilot studies will guide future research by identifying successful techniques for installation of photonic sensor networks in concrete structures and by evaluating the viability of such networks to measure ultrasonic wave propagation.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Rachel McIntyre
Grant Number: 70NANB17H164
Academic Institution: University of Maryland
Major: Mechanical Engineering

Academic Standing (Sept. '17):
Junior
Future Plans (School/Career):
Finish Bachelor's Degree and pursue graduate school
NIST Laboratory, Division, and Group:
Engineering Laboratory, Fire Research Division, Wildland-Urban Interface Fire Group
NIST Research Advisor:
Kathryn Butler and Erik Johnsson
Title of Talk:
The Effect of Wind Speed and Distance on the Speed of Fire Spread in Wildland-Urban Interface Areas

Abstract:
Over sixty thousand wildfires burn in the United States every year. These wildfires cause the most damage when they threaten communities and structures. These fires, known as Wildland-Urban Interface (WUI) fires, destroy three thousand homes annually and this number increases every year. Direct flames, radiation, and flying embers can all cause structures to ignite and spread the fire through a community. Fences, decks, vegetation, and other items on the property can also make ignition of the structure more likely.

The intent of this research is to characterize flame spread across materials in WUI regions with a focus on mulch and fences. Experiments were performed that tested mulch and fences, with and without mulch under them, placed at different separation distances from a structure and under different wind speeds. With video taken during these experiments, MATLAB was used to measure how far from the structure the flames were as time passed, to see how quickly the fire moves under certain conditions. These measurements could then be compared across separation distances and wind speeds to help make recommendations for what people living in WUI areas should do to protect their property.
### Abstract:

Machine tools are essential in the manufacturing of various components in the automotive and aircraft manufacturing industry. Degradation of machine tool linear axes has a huge impact on the quality of parts manufactured through this process. Billions of US dollars are lost every year due to degradation of machine tools during production. Currently, there are direct methods of measuring geometric errors using laser-based and other standard methods. However, these methods require the machine to be taken offline during testing. This process is time-consuming, complicated, and halts production, all of which usually equates to lost revenue making it less desirable to manufacturers.

A common degradation mechanism that can occur during machine tool operations is pitting or spalling. For this study, one rail of the linear axis testbed was mechanically degraded to simulate this form of degradation. Laser-based degradation were then separated with a technique developed in MATLAB that utilizes the various data for each run. Diagnostic metrics were then defined for use with the IMU to help inform end-users of the magnitude and location of wear and any violations of performance tolerances. The angular and translational metric values calculated from the IMU show a good agreement of over 99% correlation to the reference data, verifying how the IMU-based method can be used for degradation tracking within future smart machine tools.

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**Name:** Ashby Mullin-Conant  
**Grant Number:** 70NANB17H071  
**Academic Institution:** Doane University  
**Major:** Computer Science  
**Academic Standing (Sept. '17):** Senior  
**Future Plans (School/Career):** I am beginning research into self-tuning algorithms and I plan to pursue graduate studies in Software Engineering  
**NIST Research Advisor:** Swee Leong  
**Title of Talk:** Implementing a reusable template to model heating, ventilation and air conditioning processes

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**Name:** Grant Menu  
**Grant Number:** 70NANB17H141  
**Academic Institution:** University of South Florida  
**Major:** Mechanical Engineering  
**Academic Standing (Sept. '17):** 1st year graduate school  
**Future Plans (School/Career):** Attending the University of Florida to pursue PhD in Aerospace Engineering  
**NIST Laboratory, Division, and Group:** Engineering Laboratory, Intelligent Systems Division, Production Systems Group  
**NIST Research Advisor:** Greg Vogl & Michael Sharp  
**Title of Talk:** Diagnostics of Machine Tool Linear Axes for Smart Manufacturing

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The ASTM E3012-16 (Standard Guide for Characterizing Environmental Aspects of Manufacturing Processes) characterizes sustainability information and provides a methodology for constructing Unit Manufacturing Process (UMP) models to investigate environmental aspects of manufacturing processes. Recent results from an open competition to develop and validate UMP models revealed several limitations of the current standard. Users had trouble completely describing their models and the resulting model representations varied greatly amongst the submissions. Some possible causes of these issues include the lack of training related to ASTM E3012-16 provided to the participants and the lack of a rigorous structure presented in the originally suggested UMP information model. One eventual goal of implementing the standard is to be able to link individual models in a network to simulate factories in a virtual environment. Such a task requires the generation of models with a level of uniformity.

In response to these challenges, we propose to include template UMP representations to simplify the modeling activity for the user facilitating the creation of more refined UMP models. In this project, we tested this concept through a case study of modeling HVAC systems using the methodology outlined in ASTM E3012-16. Air conditioning processes were chosen, because almost every manufacturing system includes heating, ventilation and air conditioning (HVAC) as support. Additionally, since ASTM E3012-16 does not currently provide any guidance for formally characterizing supporting processes, understanding the feasibility of applying the standard in this manner was of interest. First, we constructed a template representation for various air-conditioning processes. Then, based on the template UMP representation, we demonstrate the creation of instance models representing individual embodiments of HVAC systems. Generation of NIST-certified templates can help to formalize the structure of UMP models, provide a schema for information exchange, and a benchmark to compare independently developed models.
**Abstract:**

Vulnerability serves as a relative measure of the propensity or predisposition of a community to be adversely affected by a shock or stress. Vulnerability is determined by factors that also affect resilience. Recent studies have focused on the importance of social factors in determining community-level vulnerability; and some studies have attempted to combine social and built factors together. While social vulnerability addresses the vulnerability of the population based on specific characteristics, it neglects the vulnerability of the built environment within which the population operates.

The Built Infrastructure Vulnerability Index (BIVI) was developed by taking factors associated with vulnerability in the built environment at the county level that are publicly accessible and determining the final composition of the important most significant factors through the implementation of principal component analysis with a varimax rotation.

In this analysis, an index of social vulnerability is correlated only loosely with the BVI. A given population may be determined to be relatively socially vulnerable, but, if their built environment is not relatively vulnerable, they may experience less stress from a hazard due to their built environment's ability to absorb some of the associated effects.

The creation of the BIVI is unique among other indices related to the built environment by including variables such as railroad nodes and access to broadband. The BVI can be used to determine the relative vulnerability of a community based upon its built environment as a means to identify at-risk areas within the United States. The use of both the social and built indices in determining vulnerability increases one's ability to identify the factors that are contributing to an area's vulnerability and effectively allocate resources to mitigate the risk associated with those factors.

However, the relative vulnerability of an area is also dependent on the probability of a shock or stress affecting the area. For this reason, a scaled value associated with the risk of a hazard occurrence in an area has been created to emphasize areas that are both vulnerable and at risk of hazard occurrence.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Jacob Pickett  
Grant Number: 70NANB17H146

Academic Institution: Worcester Polytechnic Institute  
Major: Chemical Engineering

Academic Standing (Sept. '17): Junior

Future Plans (School/Career): Pursuing a career in Chemical Engineering

NIST Laboratory, Division, and Group: Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group

NIST Research Advisor: Li Pinn Sung

Title of Talk: Who’s in Charge? Investigating the Effect of Temperature, Humidity, and UV Radiation on PET Weathering

Abstract:

The thin, translucent polymer films of Poly(ethylene terephthalate) [PET] are used in numerous applications such as protective layers on building and automobile windows, and as with any material, the phrase “how long will it last?” is often asked. While one way to determine the service life of PET is outdoor exposure, that process usually requires many weeks to months for failure to be observed. To shorten the exposure time, laboratory accelerated weathering using the Simulated Photodegradation via High Energy Radiant Exposure (SPHERE) equipment is employed. In addition to high ultraviolet (UV) light intensity, exposure conditions such as temperature and humidity can be controlled, thus their individual effect on sample degradation can be determined. PET samples were exposed to eight different conditions of high and low temperatures (70°C and 40°C), high and low humidity (70 % RH and 0 % RH), and with and without UV exposure (100 % UV and 0 % UV).

Samples were removed at different exposure times for mechanical and chemical measurements via a Tensile test and attenuated total reflection - Fourier transform infrared spectroscopy (ATR-FTIR) respectively. Changes in mechanical properties (elongation at break, toughness, yield strength, and modulus) and chemical properties (FTIR absorption values for the mass loss and oxidation) were plotted as a function of exposure time.

The accelerated weathering test indicates that high temperature and UV radiation, in both wet and dry conditions, are dominating factors in driving the degradation reactions of PET. The samples broke immediately in the Tensile test after 5 days. However, at low temperatures, humidity does affect degradation, with the more humid condition degrading more quickly. The samples exposed to 0 % UV, did not show significant degradation, neither mechanical nor chemical, within the exposure time of 17 days.

SURF Student Colloquium
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Name: Jonathan Piland  
Grant Number: 70NANB17H130

Academic Institution: University of North Carolina at Charlotte  
Major: Mechanical Engineering

Academic Standing (Sept. '17): Senior

Future Plans (School/Career): Pursue a Ph.D. in Mechanical Engineering

NIST Laboratory, Division, and Group: Engineering Lab, Intelligent Systems Division, Production Systems Group

NIST Research Advisor: Jason Fox

Title of Talk: Melt Pool Geometry Modeling and Automated Experiment Analysis for Laser Powder Bed Fusion Additive Manufacturing

Abstract:

Laser powder bed fusion (LPBF) additive manufacturing (AM) selectively melts regions of a powder bed, repeating for each layer, to create a solid object based on a three-dimensional model. Automated ex situ evaluation of the solidified melt pool (or scan track) from LPBF is needed to compare to theoretical models and in situ imaging. Due to large variations in material properties caused by the layer-wise nature of the AM process, part certification is difficult to obtain. Ultimately, part quality may be ensured during process through in situ monitoring and control. However, ex situ analysis is needed to understand anomalies and correlate them to in situ monitoring results. To build confidence in these correlations, large quantities of experiments must be analyzed, and automated solutions are needed to minimize user error and time spent on image processing. In this work, an algorithm based on the analytical solution to a moving point heat source was modified in MATLAB to compare theoretical melt pool geometries with experimental results. Additionally, optical images and height data were taken of several scan tracks deposited with varying laser velocity and power. Multiple algorithms were developed to automatically select the track width from the height data. Representative scan tracks were manually measured using the optical images and overlaid on the height data to assess the accuracy of automated measurements. Once optimized, the algorithms calculate the mean scan track width within one standard deviation of the representative mean width from the manual measurement. This, ex situ results can be correlated to in situ imaging to understand phenomena found in the monitoring data. Furthermore, the result of this work is being applied to current studies of high speed in situ monitoring systems in LPBF. Through automation, the analysis of large quantities of data and determination of correlations has been eased.
### Impact of Cybersecurity Measures on Industrial Control Systems

**Abstract:**
Industrial control systems (ICS) are integral to today’s society because of the numerous industrial processes relying on an interconnected network framework. Continuous process control (CPC) is a method employed by manufacturers to precisely control the quality and properties of a product to allow continuous manufacturing. CPC allows for continuous monitoring of the variables involved with mass production and supervising a series of actuation points to control the production process. Control systems must be able to quickly respond to changes from steady state and the controls for each process step must be tightly integrated to keep the production in operation. Each process requires different control algorithms, in our industrial chemical process simulation, modeled after the Tennessee Eastman challenge problem, there are 12 valves available for manipulation and 41 measurements available for monitoring and control.

Process industries are no place for uncertainty and risk. Companies engaging in continuous manufacturing, like oil and gas, petrochemical, water and wastewater treatment, must prevent and mitigate cyber security threats that jeopardize production operations. Despite the rising risk of cyber threats on ICS, industry has not implemented the necessary measures to prevent threats. Additionally, the impact on ICS systems in network latency, produced as the implementation of cyber security measures, have not been properly documented, specifically with the real-time requirements of ICS. This projects goal is to study the impact of cybersecurity measures on CPC. We will be looking for different network strategies to assess the impact on ICS when cybersecurity measures are implemented. The approach strategy of this project is to simulate cybersecurity effects and measure the performance impact of process control by manipulating network characteristics. Industry needs to take certain steps to protect critical assets. Taking those steps is easier with an understanding of current and future cybersecurity risks, past incidents, and knowledge of ever-changing security challenges.

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### Programmable Speed and Variable Momentum Motorized-Dynamic Bending and Calibration Machine to Test Disposable Human-Collaboration-Robotics Safety Artifacts

**Abstract:**
The outsourcing of manufacturing jobs to countries featuring low-wage labor has motivated the development of a new generation of industrial robots that can safely collaborate with human workers. Human-Collaboration-Robotics combines the endurance, repeatability, and strength of industrial robots with the dexterity and intelligence of human workers. Interfacing powerful robots with workers requires the assurance of human safety, fostering a need for safety standards that provide guidance for the development of a comprehensive risk assessment of the robot arm, its tools, its controller, and the whole operating workspace where humans might be present. Our goal is to aid in the creation of standards by developing disposable Human-Collaboration-Robotics safety testing artifacts. These artifacts will provide a means of testing the severity of bone injury to humans when they are struck by a moving robot. To test and calibrate these artifacts, we created the Motorized-Dynamic Bending and Calibration Machine (M-DyBeCaM). This machine simulates impact by striking the artifact in a three-point bending manner at a programmable speed. The M-DyBeCaM is equipped to maintain its impact speed across different weighted loads, allowing for variable momentum testing on the artifacts. This talk will discuss the development of the motor control software and circuitry required to allow for safe and accurate artifact testing.
**SURF Student Colloquium**

**NIST – Gaithersburg, MD**

**August 1-3, 2017**

**Name:** Cory Schovanec

**Grant Number:** 70NANB17H108

**Academic Institution:** Southwestern University

**Major:** Applied Physics, Mechanical Engineering

**Academic Standing (Sept. ‘17):** Senior

**Future Plans (School/Career):** Attend Washington University in St. Louis to pursue M.S. in Mechanical Engineering

**NIST Laboratory, Division, and Group:** Engineering Laboratory, Fire Research Division, Engineered Fire Safety Group

**NIST Research Advisor:** Kevin McGrattan

**Title of Talk:** NIST Vent Study: Consolidated Model of Fire and Smoke Transport (CFAST) Validation

**Abstract:**

The Consolidated Model of Fire and Smoke Transport, CFAST, is a computer program that is used to simulate the behavior and impact of fires within buildings. Developed at NIST, CFAST is a two-zone fire model that can calculate changes in temperature and smoke distribution with respect to both height and time for compartment fires. CFAST’s ability to generate this data, its short run time, and its user-friendliness make it a useful tool for fire safety and risk management. This research aims to further validate CFAST for compartments with varied natural-ventilation. To perform this task, a series of reduced-scale compartment experiments was conducted. The compartment featured a two-floor design and was constructed using gypsum board and wood studs. The floors were approximately the same size, with each floor containing eight thermocouples for measuring the vertical temperature profile.

Each experiment consisted of an enclosure with a unique combination of doors, windows, and ceiling vents. The size, shape, and time at which the vents were opened varied as well. For testing, a single propane burner was set up on the first floor. A mass flow controller was used to achieve a flow rate of approximately 1.65 sL/min. This provided a fire with a heat release rate of 2.5 kW. The temperature measurements were then compared to CFAST predictions. CFAST overpredicted the average hot gas layer temperature by 1 % and the hot gas layer depth by 3 %. This percent error remains within the uncertainty of the experiments, further corroborating the role of CFAST as a useful aid in the fire-safety decision making process.

**SURF Student Colloquium**

**NIST – Gaithersburg, MD**

**August 1-3, 2017**

**Name:** Nicolas Serrano Ragsdale

**Grant Number:** 70NANB17H164

**Academic Institution:** University of Maryland-College Park

**Major:** Mechanical Engineering

**Academic Standing (Sept. ‘17):** Junior

**Future Plans (School/Career):** Graduate School

**NIST Laboratory, Division, and Group:** Engineering Laboratory, Intelligent Systems Division, Production Systems Group

**NIST Research Advisor:** Felix Kim

**Title of Talk:** Algorithm Development for Defect Detection in X-ray Computed Tomography (CT) scans

**Abstract:**

In the additive manufacturing industry, the production of unwanted pores in products can be a critical problem. As these defects are often fracture initiation points and can negatively influence the material’s strength, their automatic detection has become an essential step in the analysis of additively manufactured products to prevent unexpected, catastrophic failures. With the availability of three-dimensional (3D) X-ray Computed Tomography (XCT) scans, researchers have been able to apply computer programs, such as ImageJ, along with thresholding techniques, whose goal is to search for dark spots in a greyscale image and completely black them out against a white background for a clear depiction of pores, to quickly evaluate the size and number of defects in these products. This research, specifically, attempts to expand and improve upon the existing thresholding methods to allow for rapid and clear detection of pores. Most currently available thresholding code consists of inspecting each individual XCT image, or slice, from the entire 3D image stack, and evaluating different areas of the slice according to user-defined threshold values. Our two-dimensional (2D) methods likewise categorize local regions of the slice differently, but also take into account the image quality by examining the image intensity fluctuation (noise). An additional step taken in the project was the implementation of this concept in a 3D environment. Though a scarcely-developed field, 3D adaptive thresholding can inspect several slices of the scan and consider the depth of pores. Both the main 2D and the 3D thresholding approaches developed have experimentally identified higher porosity levels, and in some cases, achieved a higher efficiency than the current methods. The improvement in thresholding performance from this project will provide manufacturers and researchers with a better, quicker option in analyzing the porosity levels of their product and, thus, the effectiveness of their additive manufacturing processes.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Bohan Shan
Grant Number: 70NANB17H164
Academic Institution: University of Maryland, College Park
Major: Computer Engineering
Academic Standing (Sept. ’17): Sophomore
Future Plans (School/Career): Planning on graduate studies in Computer Science or Electrical Engineering.
NIST Laboratory, Division, and Group: Engineering Laboratory, System Integration Division, Life Cycle Engineering Group
NIST Research Advisor: William Bernstein
Title of Talk: Mining the Publications Universe for Manufacturing Process Models

Abstract:
For decades, engineers have created and exploited complex models to better understand manufacturing systems. Recently, developing a standard representation of a manufacturing process model and its underlying data has become a focus area for the manufacturing community. As a related effort, a cloud-based repository to store such models is under development at NIST. One challenge for constructing such a collection of models is locating and curating appropriate content. With thousands of manufacturing papers in circulation, automated techniques that measure the likelihood of a paper containing a manufacturing process model are required. To address this need, we use a machine learning-based approach to generate statistically based evidence of a paper containing an appropriate model for curation. To build a dataset for training the algorithm, we developed a web interface to collect expert-driven tags for select research papers. Then, we employ natural language processing to predict the likelihood of a paper containing a manufacturing process model. This work provides an initial pass on the vast publication universe of manufacturing-related papers to provide more manageable tasks for populating the NIST-led repository moving forward.

Name: Stephan Smith
Grant Number: 70NANB17H098
Academic Institution: City University of New York
Major: Chemical Engineering
Academic Standing (Sept. ’17): Senior
Future Plans (School/Career): Pursue PhD in Chemical Engineering at the City University of New York
NIST Laboratory, Division, and Group: Engineering Laboratory, Energy and Environment, Indoor Air Quality and Ventilation
NIST Research Advisor: Dustin Poppendieck
Title of Talk: Application of desorption tube method to measure the mass of Semi-volatile organic compounds (SVOC) emitted from material surfaces

Abstract:
Semi-volatile organic compounds (SVOCs) are ubiquitous indoors, present in building materials (e.g., flame retardants) and household's products (e.g., antioxidants). Human exposure to some SVOCs has also been associated with adverse health conditions, including asthma, and reproductive disorders. This study focused on two common SVOCs: 1) Bis (2-ethylhexyl) phthalate (DEHP), a plasticizer in polyvinyl chloride flooring materials and 2) Tris (Chloro-2-propyl) phosphate (TCP), a flame retardant in spray polyurethane foam. Exposure to these chemicals primarily occurs indoors and currently, the health impacts are unknown. Therefore, it is important to be able to accurately determine the mass of SVOCs emitted from these materials.

Two sets of experiments were conducted using a static chamber system. The chambers are thermal desorption tubes with Tenax® sorbent depth of 15 mm. The tubes were placed on polyvinyl flooring material in an incubator at 24.9 °C for 24 h to 192 h. The mass of DEHP on the tube at a given time allows the calculation of the DEHP air-polyvinyl flooring partition coefficient. This coefficient is critical to model DEHP emission rates in the indoor environment. The experiment was repeated for TCPP in spray polyurethane foam.

The tubes were analyzed using a Gerstel TD 3.5 + thermal desorption system connected to an Agilent 6890 gas chromatograph (GC) and Agilent 5973 mass spectrometer (MS). Standard curves made from diluted DEHP and TCPP were used to back-calculate the emitted DEHP mass from vinyl chloride flooring. The same procedure was used to back-calculate the emitted TCPP mass from spray polyurethane foam.

Preliminary results show that the mass of DEHP emitted and the DEHP air-polyvinyl flooring partition coefficient is consistent with the model done by Wu et al. (2016). If successful, this technique could prove to be a useful screening tool that could develop into a standardized method.
Abstract:
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. Integrating heterogeneous functional components such as optimization, control, and simulation helps achieve Smart Manufacturing goals. The ISO 15746 (Automation systems and integration -- Integration of advanced process control and optimization capabilities for manufacturing systems) standard addresses the integration of advanced process control and optimization capabilities for manufacturing systems. The standard not only helps to ensure the integration among system components, but also the integrations across the levels of the ISA 95 (Enterprise – Control System Integration) hierarchy. A chemical process case based on the Tennessee-Eastman problem has been implemented to demonstrate the application of this standard.

The focus of this summer project was to design and implement a web-based graphical user interface (GUI) that serves as a bridge between users in level 3 and the optimization component above level 2. Process parameters were taken from the user and then saved in Extensible Markup Language (XML) format based on the XML schema developed from information models defined in ISO 15746 (Automation systems and integration -- Integration of advanced process control and optimization capabilities for manufacturing systems). The XML instance can then be used as the input to the optimizer where optimal solutions are derived. The GUI is designed for expandability; currently the focus is on production cost, but other optimization objective modules can be easily added as needed. By using a web-based application, users can access the interface from any Information Technology (IT) device and submit different inputs for the optimization problem at any location within the enterprise.
**Title of Talk:** Fused Deposition Additive Manufacturing of Cement

**Abstract:**
Various forms of three-dimensional (3D) printing, or layer-by-layer additive manufacturing, have come to the forefront as methods for quickly producing small amounts of parts with complex geometry and minimizing waste. While 3D printing made its debut as a way to form thermoplastics without the need for a mold, the technology now exists to construct cementitious structures in a similar way without the need for formwork.

As "3D printing" of construction-grade materials becomes more widespread, researchers at NIST have been analyzing the characteristics of cement that affect its "printability." By taking rheological and calorimetric measurements of cement pastes as they harden, a better idea can be obtained about how the material will behave as it sets. This information will be applied and evaluated in a large-scale cement 3D printer that is currently being developed. For practicality reasons, it is necessary to conduct small scale tests before attempting to print with the large machine.

The goal of this project was to develop and optimize an apparatus for testing the printability of cement on a small scale. An existing desktop 3D printer was modified using available software and hardware to deposit cement paste with an external pump while retaining its ability to print with plastic. Using this setup, the effects of print speed, layer height and other settings on the quality of the structures can be tested. One application of this apparatus is to print composite beam structures out of both cement and polymer lattices to simulate carbon fiber mesh reinforcement in structural concrete. Another application that was investigated was comparing the strength of printed structures to that of cast structures. Overall, this experimental setup can be used to run small tests to get an idea of the optimal conditions for cement printing before running full-scale tests.

**Name:** Thomas Winnard
**Grant Number:** 70NANB17H063
**Academic Institution:** Andrews University
**Major:** Mechanical Engineering
**Future Plans (School/Career):** Industry or Government Research
**NIST Laboratory, Division, and Group:** Engineering Laboratory, Intelligent Systems Division, Production Systems Group
**NIST Research Advisor:** Gregory Vogl
**Title of Talk:** Diagnostics via Sensors for Computer numerical control (CNC) Linear Axes

**Abstract:**
Production time, part quality consistency, and equipment reliability are crucial operational targets in the manufacturing industry that are negatively impacted by the degradation of machine tool linear axes. This project sought to achieve monitoring of axis degradation via inertial sensors. A triaxial accelerometer and a triaxial rate gyroscope are housed in a small inertial measurement unit (IMU) to sense translational and rotational motion due to micrometer-sized (μm-sized) and microradian-sized (μrad-sized) physical errors in a linear axis. The IMU travels on a linear axis carriage that is constrained to a pair of guide rails via ball bearing trucks.

An experiment was conducted in which some of the ball bearings were manually degraded without removing them from the trucks, so that nonuniform motion was experienced by the IMU when it traveled across the rails. Translational motion data and rotational motion data were collected each day for which degradation was increased. Changes were made to the LabVIEW code that controlled data collection to make motion detection extremely robust for application in real production environments. Furthermore, other IMUs were assembled for use with a mobile experimental setup that was designed and constructed for collaborators at production facilities.

All data analysis was performed in MATLAB with custom diagnostics that separated the error motions due to the ball bearings from the error motions due to the rails. Data analysis showed that the sensor-based method can be very effective in a manufacturing environment for linear axis degradation diagnostics. In the future, the method shows great potential to contribute to machine tool health prognostics to help optimize factory asset management.
Allen, Tony - ITL
Armstrong, Paul - ITL
Benz, Luke - ITL
Bringewatt, Jacob - ITL
Carrick, Cassandra - ITL
Chan, Pauline - ITL
Chen, Hong - ITL
Cyrus, Timothy - ITL
Fulton, Kelsey - ITL
Hobby, Emily - ITL
Hoyt, Christopher - ITL
Leadingham, Mark - ITL
Li, Xiang - ITL
Lin, Raymond - ITL
Linder, Rachel - ITL
McClinton, Willie - ITL
McGovern, Emily - ITL
Miller, David - ITL
Nachega, Biriningwa - ITL
Nolan, John - ITL
Rubin, Jeremy - ITL
Sarwat, Sumaiyah - ITL
Sauber, Margaret - ITL
Seese, Nicole - ITL
Srinivasan, Ananya - ITL
Strange, Sean - ITL
Thaper, Pooneet - ITL
Thorpe, Jamie - ITL
Weinberg, Theodore - ITL
Wootten, Nikita - ITL
Xiong, Xinyu - ITL
Abstract:
Shoeprint impressions are a common form of evidence found at crime scenes. Current forensic footwear impression comparison methods are subjective, and have raised questions about accuracy and reproducibility. In addition, shoeprints generally provide a weaker association between suspects and crime scenes than DNA or fingerprint evidence. A team at NIST is creating a tool to provide reliable and accurate statistical measurements to help evaluate footwear evidence. This talk focuses on just one aspect of this tool. Graph theoretic ideas are used to find an optimal mapping between crime scene shoe impressions and test impressions of suspect shoes. This provides insights on the similarities of those impressions. Given two configurations of shoeprint features, a product graph can be constructed where each vertex represents a mapping from a feature in one configuration to a feature in the other. There is an edge between two vertices if the two mappings are feasible. Cliques in this product graph represent sets of corresponding features across the two footwear impressions. Using this correspondence, the two footwear impression images are optimally aligned using rigid transformations. This alignment is useful in calculating a similarity score for the two impressions.
Name: Luke S. Benz  
Academic Institution: Yale University  
Major: Applied Mathematics  
Academic Standing: Junior  
Future Plans (Sept. '17): I plan to work as a data scientist for 2-3 upon graduation before pursuing a PhD in statistics/biostatistics.  
NIST Laboratory, Division, and Group: Information Technology Laboratory, Statistical Design, Analysis & Modeling Group  
NIST Research Advisor: Dr. Andrew Rukhin  
Title of Talk: New Procedures for Combining Results in Collaborative Studies when Reported Uncertainties are Unreliable  
Abstract: Collaborative studies, or studies in which data from several independent sources reporting a common measurement are combined, are a crucial part of nearly every scientific field. Such studies allow for analysis of larger samples of data, and thus in theory, more trustworthy results. While each independent lab/study reports its own value for the measurement in question, usually with associated uncertainty, combining the results of these individual studies can be somewhat complex. 

In addition to the variances reported by each individual study (within-study uncertainties), there may exist heterogeneity variances (between-study uncertainties) that affect each study separately. The within-study uncertainties reported by each individual study may not always be reliable, and thus are suggested as lower bounds for the true unknown uncertainties. This work seeks to test newly derived estimators for combining independent study results against existing estimators frequently employed in meta-analyses in hopes of establishing a standard technique. 

The new estimators of interest are the recently derived maximum likelihood estimators. These new estimators are compared with the existing DerSimonian-Laird estimator and a Bayes posterior mean estimator, to name a few. Each estimator can be computed on randomly generated data, with estimator efficacy evaluated using calculations of mean squared error, and confidence interval width and coverage probability. Preliminary findings suggest that the maximum likelihood estimators will outperform other existing estimators.

Name: Jacob Bringewatt  
Academic Institution: University of Maryland, College Park  
Major: Physics  
Academic Standing: Senior  
Future Plans (Sept. '17): Pursue a Ph.D. in physics and do research in quantum information theory  
NIST Laboratory, Division, and Group: Information Technology Laboratory, Applied and Computational Mathematics Division, Computing and Communications Theory Group  
NIST Research Advisor: Stephen Jordan  
Title of Talk: Substochastic Monte Carlo Versus Quantum Adiabatic Computation  
Abstract: Quantum adiabatic algorithms have garnered significant attention for their potential use in solving discrete optimization problems such as the NP-complete maximum satisfiability (MAX-k-SAT) problems. For general Hamiltonians quantum adiabatic computation is as powerful as standard quantum computation. However, most previous research regarding quantum adiabatic optimization has focused on stoquastic Hamiltonians, whose ground states can be expressed with only real, nonnegative amplitudes. As a consequence, the effects of destructive interference are not manifest. This raises the question as to whether quantum adiabatic computation with stoquastic Hamiltonians is capable of exponential speedup over classical algorithms, such as Monte Carlo.

Recent results have indicated this is not in fact the case for both path integral and diffusion Monte Carlo. However, most potential applications of quantum adiabatic computation, such as for solving MAX-k-SAT problems, use k-local Hamiltonians, and the previous counterexamples where diffusion Monte Carlo failed to efficiently simulate adiabatic quantum computing were not k-local. We demonstrate by presenting a new 6-local Hamiltonian for which SSMC fails to efficiently simulate quantum adiabatic computation that even for k-local stoquastic Hamiltonians, diffusion Monte Carlo does not provide a general method for classically simulating k-local adiabatic computing in polynomial time. This suggests that even for k-local, stoquastic Hamiltonians with no manifest destructive interference, quantum computation provides resources, such as tunneling, which allow it to outperform classical algorithms for certain types of optimization problems. 

In practice, however, diffusion Monte Carlo performs quite well on most real MAX-k-SAT problems. The success of our techniques used to develop the 6-local counterexample suggests that they can be extended to identify a good model for obtaining a deeper understanding of how quantum adiabatic and classical algorithms compare for these types of real world problems.
Humans recognize faces of their own race more accurately than faces of a different race—known as the other-race effect. A natural question arises: “Do face recognition algorithms exhibit an other-race effect?” In today’s diverse world, it is imperative that face recognition algorithms perform reliably over all races. Phillips et al., [An Other-Race Effect for Face Recognition Algorithms, 2010], looked at overall performance accuracy and showed an other-race effect for face recognition algorithms. Their work determined an algorithm developed in Western Europe or North America performed better on Caucasian faces; an algorithm developed in Eastern Asia performed better on East-Asian faces. Our current study considers the interaction between false accept and false reject rates at a fixed threshold, which is a closer model for an operational system. Experiments were performed using three data sets: (1) The Point-and-Shoot Challenge (PaSC); (2) The Good, The Bad, and The Ugly (GBU) Face Challenge; and (3) The Face Recognition Vendor Test (FRVT) 2006, (used in Phillips et al., 2010). An algorithm’s performance is more accurate when both false accept and false reject rates are lower. Conversely, when both rates are higher, algorithms are less accurate. When either rate is higher while the other is lower, one cannot unambiguously say an algorithm is better; rather there is a trade-off between changes in false accept and false reject rates. Over the three data sets, we did not find an algorithm which could be categorized as more or less accurate for Caucasian or East-Asian races. The trade-off between rates was clearly demonstrated. Additionally, as the threshold varied, so did the trade-off. These facts reveal the nuances of analyzing algorithm performance based on race and expose some of the challenges encountered while attempting to characterize their performance.
Abstract: This research aims to implement a novel approach to extract refractive index measurement using CUSUM-based algorithm for segmentation for noisy images with application to optical coherence refractometry. Cumulative sum (CUSUM) is a sequential analysis technique that is often used for change-point detection in time series analysis. CUSUM involves the cumulative sums of the deviation between each value of a sample and a sample mean. It is equivalent to the sequential likelihood ratio test (SPRT) on the mean change in most situations, therefore, even slight drift in the mean value of a sample will result in increasing or decreasing of the cumulative sums of the deviation. When the value of cumulative sum is above or below one threshold value, the change-point will be found. In this research, firstly, we use CUSUM algorithm and define the threshold value to find boundary regions in some sequence of images that was collected by NIST biophysicist Jeeseong Hwang. Secondly, we fit a two-phase linear regression model to identify the refractive angle through using the segmented package in R. The combination of the CUSUM-based image segmentation and the multiphase regression model in R, our approach will provide an automated and easy-to-use software for refractive index measurement in optical coherence refractometry.
**Title of Talk:** Unwinding the Runtime Stack: Application Runtime Analysis for Anomaly Detection Research

**Abstract:**

Intrusion detection, the runtime monitoring of a computer system with the goal of detecting malicious activity, has become increasingly important in our modern world run by computers. While anomaly detection encompasses more than software behavior monitoring and incident response, this project at NIST focuses on applying anomaly detection techniques to detect potentially malicious software runtime behavior. The model used here at NIST for detecting anomalous software behavior involves the logging of system calls and the program counter (PC) values from where these calls were made. When behavior begins to appear too anomalous, an alarm is generated.

This model is not novel, but its application with current high-performance hardware poses substantial engineering challenges. The problem is that nearly all system calls are issued through a standard library. This presents a problem when gathering PC values, since a PC value reflects the system call location in the library and not the calling context in the program. To find the PC values of the location just prior to the library call, the runtime stack must be unwound to the call location in the actual program, but the structure of the runtime stack can be obscure. The goal of this research was to create a stack unwinding application that is source code, debugging information, and program design independent. The general layout of the Unix-kernel was studied by using Ubuntu 16.04 source code. A kernel module was written to unwind the runtime stack of a running program using a model based on “normal” system calls for the behavior of the given system. The module was capable of collecting relevant information to a given system call such as a pointer to the user stack, the program counter value, and the ability to traverse the user runtime stack. The module was heavily tested for accuracy, usability, and efficiency.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Christopher Hoyt
Academic Institution: Harvey Mudd College
Major: Mathematics
Grant Number: 70NANB17H075

Name: Mark Leadingham II
Academic Institution: West Virginia Wesleyan College
Major: Mathematics / Physics
Grant Number: 70NANB17H145

### Abstract

The permanent is a function evaluated on matrices that is similar to the determinant. However, unlike the determinant where alternating signs are used within the summation, the permanent only uses positives. Because of this change, techniques that simplify the evaluation of the determinant do not extend to the permanent. In fact, while algorithms to find the determinant work in polynomial time, it has been shown that the finding the permanent of a general matrix is NP-hard. Even when the matrix entries are restricted to zeros and ones, the problem remains difficult as deterministic methods quickly become unfeasible due to their exponentially long completion time. Therefore, Monte Carlo algorithms are an attractive method for determining this quantity more quickly while retaining some level of precision.

Computing the permanent of the matrix is important in physics because the dimer covering problem reduces to computing a permanent. In addition, there are applications of the permanent within image processing and cryptography.

We applied a stratified sampling technique originally developed by Chen\(^\text{[1]}\) to the permanent approximation problem which stratifies matrices according to a sampling heuristic, and compare these results with the importance sampling algorithm developed by Beichl and Sullivan\(^\text{[2]}\). Experiments indicate a greatly reduced variance.


**Title of Talk:** Software-Based Methodology for Network Precision Time Synchronization  

**Abstract:**  
Synchronization is used in a wide range of applications. One important application of synchronization is in the power system. The power grid is considered to be a very complex and interconnected system — a failure in one part can potentially affect a large area of the grid. In order to fully understand and control complex systems like the power grid, precise timing is essential for the operator to be able to monitor the system in real time and diagnose the problems when they occur.  

The Global Positioning System (GPS) is a common use to insure the precision of time. However, while GPS provides precise time, it has a higher cost and is sometimes inaccessible. Utilities and operators are looking for new synchronization solutions that are easier to implement and also have the same level of accuracy as GPS. One new emerging solution is IEEE 1588 Precision Time Protocol (PTP), a packet-based synchronization that works over standard communication protocols.  

The subject of this project is to develop a software method to analyze time offset using PTP packets information and to investigate if this method can measure time error. In this study, two delay measurement mechanisms were compared — End-to-End and Peer-to-Peer. We used Wireshark to capture the network traffic of the subject PTP packets in the capture file, and then the delay is calculated using this generated data. The delay was then filtered out based on the different mechanisms. By using moving average, we were able to filter out white noise and narrow down the offset of peer-to-peer by the order of a few microseconds.
**Abstract:**

NIST’s OOF3D software simulates mechanical, thermal, and electrical stressors on physical microstructures. A typical microstructure contains multiple materials and complex features such as cracks, grains, and pores. The user uploads a three-dimensional image of a microstructure, assigns properties to the materials pictured, overlays tetrahedral finite elements, and creates a boundary-value equation. OOF3D solves for the displacement, temperature, or voltage of each element using finite element analysis.

The edges of the finite elements make up a net-like structure called a skeleton, and the vertices of the elements are called nodes. OOF3D has many skeleton modifiers that assist the user in creating well-formed elements. The OOF3D solver’s results are most reliable when elements contain only a single material and have a nearly regular shape. My project was to implement the Relax modifier using Python and C++. This modifier existed in OOF2, the two-dimensional predecessor of OOF3D, but needed to be added to OOF3D. It temporarily assigns two properties to every element and uses the solver to find the resulting displacement of each node. One property favors the formation of regular tetrahedra, and the other favors elements that contain a single material.

Guided by code from the OOF2 Relax method and existing OOF3D skeleton modifiers, I wrote a minimally functional version of Relax for OOF3D. To improve versatility and avoid exceptions, I added a feature that automatically scales down the node displacement if needed. This prevents the formation of illegal elements, which are tetrahedra whose four vertices are coplanar.

The primary advantage of Relax is that it works with the entire skeleton at once instead of modifying one node or element at a time. When multiple nodes need to move together to obtain the best skeleton, using Relax before another modifier produces a much better skeleton than just using the other modifier alone.

**Title of Talk:**
Implementing the Relax Algorithm in OOF3D

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**Abstract:**

TREC Video Retrieval Evaluation (TRECVID) is an independent evaluation that stemmed from the TREC conference series who’s initiative is to support research in information retrieval by offering collections of data, uniform scoring measures, comparing results, and connecting organizations interested in working together. Multimedia event detection is a growing technology and clearly defined metrics will help contributors to compare and evaluate their algorithms. One of the TRECVID tracks is the Multimedia Event Detection (MED) evaluation, which provides an open forum to catalyze the advancement of event detection systems.

The MED evaluation analyzes event detection technologies with the ability to quickly and accurately search large datasets of multimedia clips based on user defined queries. These systems are evaluated primarily based on Mean Inferred Average Precision, and the speed of different processing modules. The evaluation defines a set of events which consist of complex directly observable activities involving people interacting with other people and/or objects. These events are precisely defined and vetted to avoid semantic or interpretative complications.

This year’s MED17 evaluation will be changing from the previously labeled HAVIC Progress set to a newer unlabeled subset of Yahoo’s YFCC100M dataset. For the purpose of gathering new events and examples, searching through new dataset manually was infeasible due to the YFCC100M collection being unlabeled. A solution to this problem was the utilization of previous year’s event detection systems to rank the items in the dataset. This reduced the large search space into manageable subsets, where the most useful videos were brought to the surface. These subsets could then be manually probed for new events and examples. Along with the new dataset, this year’s MED17 will be adding 10 new Ad-Hoc events and this reboot will give more breadth to evaluation, allowing for a larger variety of tests to more accurately see the full extent of the state-of-the-art systems.

This project and the right to use the data mentioned has been reviewed by ITL-17-0025.
**Title of Talk:** Geometric Characterization of Features for Forensic Footwear Impression Comparisons

**Abstract:**

Forensic footwear analysis involves the comparison of shoeprints found at crime scenes with test prints of known shoes. When examining shoeprints, it is important to have an objective way to characterize the patterns and features found in the impression in question. Many of these features resemble common geometric shapes. The similarities between the features and such shapes can be used to classify the feature in an impression. Our goal is to create a scoring system whose input is the user-marked boundary of a feature. This scoring system will use geometric methods to calculate the distance of this boundary from a set of ideal shapes and provide a numerical score related to the distance to each ideal shape.

This scoring system is based on the Jaccard distance, a metric that is based on the intersection and union of two finite sets, and on finding a best-fitting shape of each of the set of ideal shapes to the given boundary. First, an initial estimate for a best fitting shape is found based on the boundary points and properties of the shape in question. Then, the fmin function from Python’s scipy.optimize library is used to minimize the Jaccard distance between the boundary and candidate shape and the best fitting shape is found. The Jaccard distance between the best-fitting shape and the boundary becomes the distance from the boundary to that shape.

Once these methods are implemented for eight basic shapes (circle, ellipse, triangle, square, rectangle, pentagon, hexagon and quadrilateral), the scores taken from each of these shapes will form a profile for the feature in question. Features classified using this method can then be compared between impressions and be used to find matches between crime scene impressions and test prints.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Biringingwa Nachega
Grant Number: 70NANB17H085

Academic Institution: Montgomery College
Major: Computer Science

Academic Standing (Sept. ’17): Sophomore

Future Plans (School/Career): Pursuing a career in Computer Science

NIST Laboratory, Division, and Group: Information Technology Laboratory, Software and Systems Division, HQ

NIST Research Advisor: T N Bhat

Title of Talk: Re-building user friendly webpages to utilize NLP generated terminology for efficient searching

Abstract:
The main purpose of search engines is to help people find pertinent information without too many mouse clicks. Most of today’s search engines offer suggestions to people based on what they type in a search box. These suggestions are often derived from popular keywords and sentences related to what people have searched in the past. Searching scientific databases can be an even more daunting task than searching general purpose databases. The need for precision and convenience is much greater while doing scientific research, and time is always critically important. This project re-develops previously created webpages to improve their usability. It uses the terms generated by root and rule based approach described elsewhere. Some of the new features of the re-developed webpages are (1) an auto-suggest that high-lights the search terms; (2) summary of the results where search terms are high-lighted; (3) a Web service to create terms from uploaded data. These new features increase the speed of finding relevant scientific information contained in document repositories available at the National Institute of Standards and Technology (NIST).

SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: John Nolan
Grant Number: 70NANB17H167

Academic Institution: University of Maryland – College Park
Major: Mathematics and Physics

Academic Standing (Sept. ’17): Sophomore

Future Plans (School/Career): I plan to attend graduate school in mathematics and pursue a career in mathematical research.

NIST Laboratory, Division, and Group: Information Technology Laboratory, Software and Systems Division, Cyber Infrastructure Group

NIST Research Advisor: Spencer Breiner

Title of Talk: String Diagrams and You: Translating User Actions into Categorical Structure

Abstract:
The mathematical discipline of category theory abstracts the structure of systems and processes, allowing for lucid reasoning that is reusable across fields. Categorical logic has been used to simplify and stimulate research in topics as disparate as quantum mechanics, topology, and database management. The goal of this project is to increase the reach and utility of category theory by creating a web-based application for the creation and manipulation of categorical string diagrams.

String diagrams enable users to prove theorems and specify computations by doing no more than dragging wires and beads (representing resources and processes) around. They encapsulate the logic of category theory in a rigorous pictorial toolkit that requires little formal training to use.

Much of this project involves working through use cases for the software. Each use case tracks the user interactions, on-screen representations, and computational parse trees for a specific string diagram throughout its creation.

Challenges in creating the software center around translation between the graphical, computational, and mathematical representations of processes. There is no one-to-one correspondence between diagrams and parse trees, so parse trees cannot be recovered perfectly from their diagrams. To resolve this, the software builds the parse tree in tandem with the diagram so that the user’s choices when making the string diagram control the parse tree’s structure. Furthermore, one broad user action may correspond to multiple parse tree changes. The software handles this by splitting such actions into smaller sub-actions, which are under the user’s control.

In this talk, I will discuss the fundamental ideas of category theory and describe the software created. I will also describe the difficulties that arose when planning the software and outline how we devised solutions to these problems. These will be explained with examples from computer science, chemistry, and other sciences.
**Title of Talk:** Development of an Image Processing Toolbox for the CAVE

**Abstract:**
Software testing minimizes errors that are introduced as a system develops. A CAVE Automatic Virtual Environment (CAVE) is an immersive virtual reality environment that consists of both hardware and software systems that jointly produce the images that are viewed. Hardware tests are performed separately and ensure that the hardware is running as expected before the software tests are run. In our CAVE, the graphics rendering is performed using OpenGL; however, the OpenGL standard does not guarantee that the pixels displayed will be exactly the same from run to run, or with different GPUs, or with different drivers. The challenge is to determine if a software test has passed or failed when the baseline and generated images are different.

Currently, we have a suite of software tests and a single evaluation program, compare-binary. Compare-binary returns the number of pixels that are different between each baseline image and the comparable image generated with the current test. It is desirable to have more information on the tests that do not return zero different pixels.

We have developed a suite of algorithms that will quantify and visualize the differences between baseline and currently generated images. The utilized image processing techniques span approximately four main types: measures of statistical distance/divergence, image transformations, mathematical morphology, and image segmentation. Statistical distance/divergence allows for comparison of the dissimilarity of sRGB color channels. The image transforms enable feature extraction. Similarly, mathematical morphology can be used to detect edges and highlight the overall structure of an image. Lastly, image segmentation is a useful technique for identifying objects.

**Title of Talk:** Metrology for Software

**Abstract:**
Metrology is the science and technology of measurement. Similarly, software metrology is the scientific study of software metrics where software metrics are tools for anyone involved in software engineering to understand the varying aspects of the code base, and the project process plus progress. Over the years, many software metrics have evolved. However, these metrics have never been or organized into a proper (official) system of quantities. Hence, the aim of this project is to develop a coherent standard for software metrics and its future. The ultimate goal is to obtain a well refined catalog/database for a coherent standard for software metrics that will help in the measurement of software and can be used on a global level just like the physical measurement standards.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Margaret Sauber
Grant Number: 70NANB17H169
Academic Institution: University of Maryland – College Park
Major: Mathematics
Academic Standing (Sept. ’17): Senior
Future Plans (School/Career): Pursuing a career in applied mathematics and eventually attending graduate school for mathematics or computer science
NIST Laboratory, Division, and Group: Information Technology Laboratory, Applied and Computational Mathematics Division, Immersive Visualization Laboratory
NIST Research Advisor: Judith Terrill, Steve Satterfield
Title of Talk: Monitoring Super Computing via Visualization
Abstract:
NIST does research into the flow of dense suspensions of cement paste, mortar, and concrete. Using knowledge gained from this research, NIST is producing standard reference materials for these materials. Numerical simulation used for part of this work often requires weeks or months of runtime on high end supercomputers. Analysis of the computation performance is necessary early and often to ensure a successful outcome. To provide researchers this ability through visualization, we created the Monitor, Explore, and Review software with the Immersive Visualizations (MERSIV) toolkit. A running simulation will periodically store data into a collection directory, and then users will utilize the MERSIV tools to monitor how the computation is doing. MERSIV is based upon the NIST High End Visualization (HEV) system. Researchers will be able to display and analyze their findings in the CAVE, which is an immersive virtual reality environment. The immersive experience allows for deeper exploration and review of the data.

Some of the MERSIV tools include animation creation with flipbooks, and creation of fundamental timeline paths that can be applied to multiple simulations. Combined, these two tools will allow a complete fly through experience of a dynamic model. There is also a utility to visualize vector fields. In the case of the cement paste, mortar, and concrete flow, this will be useful in understanding patterns in velocity data.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Nicole Seese
Grant Number: 70NANB17H154
Academic Institution: Millersville University
Major: Computer Science
Academic Standing (Sept. ’17): Recent Graduate
Future Plans (School/Career): Pursue a graduate degree in bioinformatics
NIST Laboratory, Division, and Group: Information Technology Lab, Computer Security Division, Cryptographic Technology Group
NIST Research Advisor: Kerry McKay
Title of Talk: Exploring the Utility of the PAQ4 Data Compressor for Estimation of Min-Entropy
Abstract:
Entropy sources provide the random material needed by cryptographic systems to generate secret keys. In order to ensure the security of a cryptographic system, one must determine how often an attacker would be able to correctly predict the output of the entropy source. This is measured in bits of entropy. Min-entropy serves as a conservative measure of entropy and correlates to the difficulty of guessing outputs of an entropy source correctly.

Min-entropy can be estimated using predictors, which predict the next bit to be output by the entropy source based on models built from the previously output bits. By determining the number of outputs correctly predicted and the longest run of correctly predicted outputs, one can estimate the min-entropy of a source.

Data compression, which aims to reduce the number of bits required to represent information, also uses predictors to achieve its goal. The PAQ family of data compression algorithms use a set of weighted submodels to predict the next bit read in from a file. This project focused on computing the abovementioned metrics for the PAQv2 data compressor to determine its suitability for min-entropy estimation. The PAQv2 source code was modified to allow the data compressor to work with integer data and record metrics for each of its nineteen submodels, as well as the final weighted model. Metrics were computed for randomly generated datasets pulled from four families of probability distributions.
One of the challenges within Natural Language Processing is generating taxonomies exhaustive enough for term searches over indexed documents. Topic Modeling methods are most commonly used for many text-mining tasks, such as indexing, searching, and retrieval. Word2Vec is a topic modeling approach developed by Google which produces word embeddings from a given vocabulary of terms. It is a two-layer neural network model for learning relationships between words in an unsupervised fashion. The computation efficiency of Word2Vec model relies on size of the input vocabulary. Additionally, Word2Vec has no control over the vocabulary other than building the model based on the given vocabulary. The vocabulary given to the model is generated from n-gram representation which is generated from a co-occurrence of words for a given window size. On the other hand, the root and rule based method extracts compound terms that are semantically meaningful n-grams as opposed to traditional n-gram generation that is combinatorial. Thus, the size of vocabulary generated from root and rule based method is small compared to that of the traditional method.

This project focuses on leveraging the computational performance of Word2Vec topic model using root and rule based terms. To illustrate this potential, two separate Word2Vec topic models were built on text documents using general n-grams and terms generated from root and rule based method. The Word2Vec model generated from root and rule based terms is computationally less expensive as compared to the Word2Vec model with general n-grams. This result can be expected since the root and rule based method extracts specific phrases using a set of rules based in natural language. Factors that were used to compare these two models were computational time, vocabulary size, and extracted term clusters. The results from these models will be discussed in the presentation.

Applications of this project include integrating these models into the NIST INet database to further improve search terms for efficient document retrieval.
Machine learning (ML) is a branch of artificial intelligence that aims to develop computer programs which change iteratively based on exposure to data and experience. An ML program’s goal is to extract insights from the information it receives without explicit programming instructing it on how to do so. Currently, data scientists must manually design, implement, and improve ML models; a workflow which has limited the technology’s availability due to the time and expertise required. The DARPA Data-Driven Discovery of Models (D3M) program aims to address this by automating much of the ML process, allowing data scientists to utilize their time more efficiently and others access to powerful ML techniques.

NIST’s role in the D3M program is to design and implement the evaluation of systems submitted by performers, namely university and industry teams. This includes reviewing each submission, creating an end-to-end plan for testing, and preparing the automated infrastructure to run and evaluate the full array of systems. The base Technical Area 1 (TA1) submissions, called primitives, are software units that perform a particular task in the ML pipeline and are to be discovered and integrated automatically by more advanced automated and semi-automated ML pipeline creation systems (TA2 and TA3, respectively) in solutions to applicable challenge problems.

Among my contributions to the NIST D3M program has been the development of test plans for TA1 primitives. The test plan design process consists of studying the primitive submission and corresponding research papers, following-up with performers, developing a relevant challenge problem, identifying an applicable dataset, and determining an appropriate evaluation metric to score the primitive’s performance. Additionally, I have worked to develop a framework which enables TA2 and TA3 systems to query the D3M schema database at runtime in order to access the various schemas necessary and discover primitives to incorporate.

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A wide range of products today are being designed for interconnectivity and communication, either among separate devices or between various sensors in a single device. While it may seem like this future of “smart” technology can’t come soon enough, such interconnectivity does present some challenges. The technology used to build these devices is evolving faster than the security protocols needed to keep them from being vulnerable to attack. Security concerns, such as confidentiality and data integrity (the guarantee that received data has not been tampered with during transmission), are often addressed in products such as laptops and smart phones using large encryption and hashing algorithms. Such algorithms were originally designed for use on workstations and servers. A different approach must be taken to handling these security challenges in devices controlled by microcontrollers because they do not have as much processing power as larger devices. This power deficit in microcontrollers is insufficient to implement such complex algorithms. The goal of this project was to investigate confidentiality and data integrity concerns could be mitigated on a system of two microcontroller nodes communicating via a Control Area Network (CAN) bus. For this project, a “lightweight” encryption algorithm called “SKINNY” was implemented in order to provide authenticated encryption for the messages sent between the two performers, namely university and industry teams. This includes reviewing each submission, creating an end-to-end plan for testing, and preparing the automated infrastructure to run and evaluate the full array of systems. The base Technical Area 1 (TA1) submissions, called primitives, are software units that perform a particular task in the ML pipeline and are to be discovered and integrated automatically by more advanced automated and semi-automated ML pipeline creation systems (TA2 and TA3, respectively) in solutions to applicable challenge problems.

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Title of Talk: System Call Anomaly Detection Using Artificial Neural Networks

Abstract:
There is a growing need to protect computer systems from constantly evolving threats. One method of identifying threats is anomaly detection. The objective of anomaly detection is to utilize patterns in normal behavior to detect deviations that might signal the onset of malicious activity. My goals were to train neural networks capable of detecting abnormal behavior and to evaluate the performances of different neural network architectures.

In this project, I analyzed behavior at the system call level. I examined system call data from both attacks and normal use to determine what aspects of the system calls best differentiate between normal and abnormal behaviors. After analyzing the data using entropy calculations, I concluded that working with sequences of system calls would be the most effective method of extracting information about normal behavior.

To generate a model for detecting anomalies, I developed deep recurrent neural networks that learned from known normal behaviors. Ordinarily, classifying behavior as normal or abnormal can be done with a straightforward classification neural network. However, due to the inherent rarity of abnormal data and how different new attacks can be, classification becomes difficult. Thus, I implemented networks using autoencoding and prediction that only need to train on normal behavior. The effectiveness of the different implementations will be discussed during the presentation.
<table>
<thead>
<tr>
<th>Name: Xinyu Xiong</th>
<th>Grant Number</th>
<th>70NANB17H098</th>
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<tbody>
<tr>
<td>Academic Institution: The City College of New York</td>
<td>Major: Computer Science</td>
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<td>Academic Standing (Sept. '17):</td>
<td>Senior</td>
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<td>Future Plans (School/Career):</td>
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<td>NIST Laboratory, Division, and Group:</td>
<td>ITL</td>
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<td>NIST Research Advisor:</td>
<td>Vincent Hu</td>
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<tr>
<td>Title of Talk:</td>
<td>ACCESS CONTROL RULE LOGIC CIRCUIT SIMULATION (ACRLCS)</td>
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Abstract:
AC Rule Logic Circuit Simulation (ACRLCS) system provides an automatic method through the construction of a simulated logic circuit that simulates access control policy rules such that allows real-time detection of policy rule faults including conflicts of privilege assignments, leaks of information, and conflicts of privilege inheritance assignments. My research is to analyze and compare performances for different access control verification methods including ACRLCS in term of computing complexity, in addition I enhanced ACRLCS capabilities by implementing GUI (Graphic User interface), dynamic rule editing, and more efficient verification functions.
Afolabi, Toyosi - MatSci/NCNR
Arnheiter, Edward - MatSci/NCNR
Arputhasamy, Cyrene - ChemBio
Bao, Annie - MatSci/NCNR
Blick, Emily - MatSci/NCNR
Brake, Alexis - MatSci/NCNR
Brignac, Kayla - ChemBio
Brooks, Sydney - MatSci/NCNR
Brown, Emily - MatSci/NCNR
Butt, Moiz - MatSci/NCNR
Campanella, Anthony - MatSci/NCNR
Cavazos, Omar - MatSci/NCNR
Chang, Eddie - MatSci/NCNR
Chen, Andre - MatSci/NCNR
Chen, Shuzhen - MatSci/NCNR
Chung, Hionu - MatSci/NCNR
Collett, Cayla - ChemBio
Cook, Chloe - MatSci/NCNR
Devers, Rachel - MatSci/NCNR
Dharmaraj, Vishnu - MatSci/NCNR
Ericks, Andrew - MatSci/NCNR
Farrar, Alison - MatSci/NCNR
Filteau, Jeremy - ChemBio
Finlay, Ethan - ChemBio
Francis, Deandra - ChemBio
Freilich, Justina - MatSci/NCNR
Garatsa, Ray Shimry - MatSci/NCNR
Garringer, Brady - MatSci/NCNR
Gayle, Andrew - MatSci/NCNR
Ghorab, Salma - ChemBio
Giufre, Rosario - MatSci/NCNR
Hong, Lisa - MatSci/NCNR
Jiao, Sally - ChemBio
Jordon, Matthew - ChemBio
Kaneshige, Nathaniel - MatSci/NCNR
Knobloch, Emmie - ChemBio
Lech, David - MatSci/NCNR
Leontyev, Dmitry - ChemBio
Liu, Kevin - MatSci/NCNR
Lucas, Laura - ChemBio
Luperico, Adrianna - MatSci/NCNR
Mandavia, Rohit - MatSci/NCNR
McIntyre, Sean - MatSci/NCNR
Mullin, Kathleen - MatSci/NCNR
Musteata, Elena - ChemBio
Negron, Raul - MatSci/NCNR
Neves, Paul - MatSci/NCNR
Ng, Daniel - MatSci/NCNR
Nguyen, Ai - ChemBio
Pretti, Evan - ChemBio
Quezada, Ramsess - ChemBio
Rahimi, Benjamin - MatSci/NCNR
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Smith, Samuel - ChemBio
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Su, Katherine - MatSci/NCNR
Tatman, Eric-Paul - MatSci/NCNR
Torsi, Riccardo - ChemBio
Tronstad, Zachary - MatSci/NCNR
Underwood, Ryan - MatSci/NCNR
Vega, Miguel - MatSci/NCNR
Wade, Matthew - MatSci/NCNR
Wigham, Caleb - MatSci/NCNR
Wilson, Shaleaghk - MatSci/NCNR
Wu, Thomas - MatSci/NCNR
**Name:** Toyosi Afolabi  
**Grant Number:** 70NANB17H084  
**Academic Institution:** Miami Dade College  
**Major:** Chemistry  
**Future Plans (Sept. '17):** Pursuing a bachelor's degree in Chemistry and attend pharmacy school to obtain PharmD.  
**NIST Laboratory, Division, and Group:** Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Research Group  
**NIST Research Advisor:** Daniel W. Siderius  
**Title of Talk:** Collection and Organization of Adsorption Isotherms for Standard Reference Use  

**Abstract:**  
Adsorbent materials play a significant role in the nation's science and technology. Activated carbons, zeolites, and metal organic frameworks are examples of materials being used in studies of adsorption. These materials are present in physical and chemical systems and are commonly used in industrial applications such as gas storage, gas purification and separation, and heterogeneous catalysis as well. There are few standard data resources for adsorption, making interlaboratory comparisons difficult. NIST has established a database that will allow researchers to access and compare adsorption data and is expanding the database system so scientists, engineers, and researchers can use it as a guide in their work. In this research, we reviewed journal articles to collect single component and multicomponent isotherms. We extracted and digitized the isotherms from the articles and uploaded them into the database. Additional work was required for multicomponent isotherms because the compositions of the gases necessitates the inclusion of extra information. Some of the isotherms had minor mistakes, such as the scaling and the temperature not being given, that were corrected.

**Name:** Edward Alexander Arnheiter  
**Grant Number:** 70NANB17H069  
**Academic Institution:** Colorado School of Mines  
**Major:** Metallurgical and Materials Engineering  
**Academic Standing (Sept. '17):** Senior  
**Future Plans (School/Career):** Graduate school for materials science.  
**NIST Laboratory, Division, and Group:** Materials Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group  
**NIST Research Advisor:** Feng Yi  
**Title of Talk:** Analyzing Surface Chemistry of Thin Film Platinum via Nanocalorimetry  

**Abstract:**  
We have analyzed a mysterious platinum thin film surface chemistry reaction using nanocalorimetry. Nanocalorimetry is a technique to determine phase transitions and chemical reactions of very small samples of materials. Microfabricated nanocalorimeter sensors can make thermal measurements on samples ranging from micrograms to nanograms with high sensitivity at the nJ/K range and heating/cooling rates up to 10^6 K/s. Nanocalorimetry can measure some chemical/physical processes that were previously impossible to detect.

The mysterious exothermic peak at ~ 300 °C is observed when the platinum thin film is heated in air, but appears endothermic when heated in vacuum or disappears when tested in gases such as argon or nitrogen. If retested soon thereafter, the peak does not reappear, but will return after hours of exposure to air. It is conceivable the peak is associated with oxidation, decomposition, desorption, or catalytic activity, but none of these explanations alone seem to account for all the observations. This presentation will report on the various possibilities and the measurements made under different environments to evaluate the appearance and disappearance of this mystery peak and summarize the implications.
**Title of Talk:** Parallelization of Atom-Based Molecular Properties using MPI

**Abstract:**

The development of circulating cell-free tumor DNA reference material for HER2 copy number measurements in liquid biopsy.

Since the amplification of the HER2 gene occurs in about 25% of breast cancers and 20% of gastric cancers, the accurate measurement of HER2 copy number is important in providing cancer diagnostic and prognostic information. The NIST Standard Reference Material (SRM) 2373 was developed for HER2 copy number measurements in genomic DNA from cancer tissues. Recent developments in deep sequencing and digital PCR (dPCR) techniques support the clinical validity of circulating cell-free tumor DNA (ctDNA) as a 'liquid biopsy' in human cancer. However, the development of non-invasive methods to detect and monitor HER2 amplification continues to be a major challenge because of the low abundance of ctDNA in the blood and lack of assay validation and reference materials. The aim of this study is to develop a ctDNA reference material for HER2 copy number measurements in the blood of cancer patients or liquid biopsy.

A bacterial artificial chromosome (BAC) that contains the entire HER2 gene was used for the preparation of HER2 gene spikes. After extracting the plasmid from E. coli, the composition and size of the construct was confirmed by PCR, DNA fragment analysis and partial Sanger sequencing. The HER2 copy number was quantified by droplet digital PCR (ddPCR). HER2 copy number was expressed as the ratio of HER2 gene copy number to the copy number of three reference genes. Both the HER2 BAC plasmid and background normal human genomic DNA from GM24385 were fragmented into pieces of about 160 bp in length to mimic the ctDNA size in the blood DNA sample by Covaris sonication. Reference materials with HER2 copy number ratios of 1.0, 1.2, 1.5, 2.0, and 4.0 will be prepared and characterized by dPCR and next-generation sequencing (NGS). These developed materials are ctDNA reference material candidates for HER2 copy number measurements. Future interlaboratory study of these reference materials will be performed and validated for utility and communicability. The success of ctDNA reference materials for HER2 copy number measurements will enable early detection, treatment selection, surveillance of disease progression and response to treatment in breast and gastric cancer via liquid biopsy.
**Title of Talk:** The Role of Detergents in the Crystallization of Membrane Proteins from Lipidic Cubic Phases

**Abstract:**

In meso crystallization is commonly used to crystallize membrane proteins prior to structural characterization by x-ray crystallography. Following the isolation of cell membranes, detergents are added to the sample, solubilizing the target protein and forming protein-detergent complexes. By homogenizing the protein-detergent solution with an appropriate lipid, the protein can be incorporated into lipidic cubic phases, which are three-dimensional networks of lipid bilayers. In the cubic phase, the protein can remain active and in its native conformation as it freely moves around within the bilayer. After the addition of precipitant, protein crystal growth can occur directly from the lipidic cubic phase. Detergents are necessary for initial protein solubility, but the importance of detergent identity on lipidic cubic phase crystallization remains unknown. Throughout the experimentation, the membrane protein Bacteriorhodopsin was used as a model system due to its stability and crystallization propensity. This experiment was designed to compare crystallization success in bacteriorhodopsin over a large span of detergents ranging from nonionic detergents with varying carbon chain lengths and head groups to stronger zwitterionic detergents. In addition to analyzing the differences between detergents in crystallogenesis, small-angle neutron scattering (SANS) was used to determine whether detergents form phase-separated structures in the lipidic cubic phase under typical crystallization conditions (with and without precipitant). Alternatively, detergents may remain “dissolved” or dispersed in the lipid bilayer, in which case their specific identity is less likely to be important to crystallization. Through these experiments, we will identify the effect of detergent properties on their success in protein crystallization.

**Title of Talk:** Evaluating the role of fiber degradation in affecting the aging characteristics of carbon nanotube based hierarchical composites

**Abstract:**

Carbon Nanotubes (CNTs) have excellent thermal, mechanical, and conductive properties. When grafted onto fiber surfaces for use in polymer-matrix fiber reinforced composites (FRP), CNTs have been found to introduce new properties such as electrical conductivity. When CNT functionalized FRPs (CNT-FRPs) are deployed for commercial (aerospace and structural) applications, environmental aging caused by exposure to moisture and temperature variations is of primary concern. A lack of understanding of these properties and a growing demand for the commercialization of nanoengineered CNT-FRPs has necessitated further investigation of the lifetime of these novel materials. In unmodified FRPs, exposure to hydrothermal conditions (60 °C and water) reduces the composite strength by half in only a week. From literature studies, it is well known that the alumina fibers (Al₂O₃) can rapidly react with water to form crystal complexes, bayerite (γ-Al₂O₃) and boehmite (γ-AlO(OH)). This reaction may be responsible for the loss of strength in these materials. CNT-modified FRPs are more durable, but the reaction of alumina with water at the fiber interface in the composite is not clear. This work focuses specifically on the effect of water and temperature on alumina fibers with the goal of characterizing the extent and rate of reaction of alumina fibers and water. To investigate this, bare alumina fibers were soaked in water at 60 °C for various lengths of time (up to 15 days) and then analyzed to monitor the hydration reaction. Our analysis utilized thermogravimetric analysis (TGA) to measure the loss of the hydration products and scanning electron microscopy (SEM) to visualize hydration products on the surface of the fibers. We show the rate at which the reaction occurs to predict the contribution of alumina hydration to composite failure.
**Title of Talk:** Polymer Identification of Coastal Marine Debris Plastics in the Main Hawaiian Islands by Fourier Transform Infrared Spectroscopy to Determine Sources

**Abstract:**

Plastic materials are a prevalent form of marine debris contributing to a growing environmental pollution crisis. Coastal plastics throughout the main Hawaiian Islands were collected for polymer identification using Fourier Transform Infrared Spectroscopy (FT-IR) analysis. Eight beaches were sampled in triplicate using systematic transects on four different islands, generating more than 3,000 pieces of macroplastics (> 1 cm). The primary polymer present was polyethylene, comprising approximately 60% of pieces and 50% of mass. Polymer composition varied among beaches, indicating differences in land- vs. ocean-based sources. The results support our hypotheses: windward beaches have more debris mass, and more from ocean sources, than leeward beaches; surrounding population density and land use explain some variability; and pieces from ocean-based sources show greater physical weathering which can be observed by an abundance of carbonyl groups present in the FT-IR spectra due to oxidation. This chemical technique can provide much needed information to policy makers to focus efforts on solutions to this pollution crisis.
**Abstract:**

An increasing amount of materials science data and software is being generated and made available to the public in order to facilitate research. However, the difficulty of finding these resources can prevent their effective utilization. The NIST Materials Resource Registry (NMRR) was created for the purpose of making those resources easier to find by materials scientists. The NMRR, still in its early stages with approximately 200 resources, will act as a catalog for other high-level materials science resources such as organizations, software, and other databases, thereby making preexisting resources easily discoverable and usable by a greater number of materials scientists.

This project aimed to analyze and visualize the overall contents of the NMRR in order to guide its development in the future by identifying vocabulary that may need to be refined, which types of resources are most represented in the system, and areas to populate more fully. Appropriate vocabulary for the resources will facilitate finding them, and modifying the registry to be more user-friendly will encourage other groups or individuals to register their own resources. This project culminated in a Jupyter notebook which can be run over time in order to catalog modifications, if needed, are required to return the system to design specifications. Changes that bring the system up to industry standards are also needed especially in terms of making the system reliable, safe, and easier to maintain.

Multiple experiments were developed to test the reliability of the system during a major scram. Due to the limited amount of time and reactor shutdown coordination, one test was conducted for pressure drop to check for undesirable pressure changes, leaks, confinement and equipment monitoring. The obtained data can then be used to make modifications to the system by implementing tightening connections, replacement of valves, or modifying the air source to provide accurate air.
### Anthony Campanella

**Name:** Anthony Campanella  
**Grant Number:** 70NANB17H137  
**Academic Institution:** University of Delaware  
**Major:** Chemistry  
**Academic Standing (Sept. ’17):** Senior  
**Future Plans (School/Career):** Attend Graduate School for a Ph.D. in Chemistry  
**NIST Laboratory, Division, and Group:** NIST Center for Neutron Research, Neutron Condensed Matter Science Group  
**NIST Research Advisor:** Ben Trump & Craig Brown  
**Title of Talk:** CO₂ Adsorption in Heterometallic Metal-Organic Frameworks  
**Abstract:**

Metal-organic frameworks (MOFs) are three dimensional porous structures composed of organic ligands bound to a metal center. MOFs possess extremely high surface areas; hence why gas adsorption has been the most researched application, focusing on sequestration and separation of small molecules like methane and CO₂. This has the potential to greatly change the way fuels are stored and offer solutions to mitigate the release of greenhouse gases to the atmosphere.

A recent publication asserted that certain mixed-metal MOFs, bridged by the ligand 3,3',5,5'-azobenzeneetetraacarboxylic acid (ABTC) produced exceptionally high CO₂ uptakes, as well as a large range of isosteric heats of adsorption. Our goal was to determine the atomistic mechanisms giving rise to these results through neutron powder diffraction and gas adsorption techniques. Unlike X-rays, neutron diffraction is particularly useful in characterizing MOFs due to its ability to accurately detect lighter elements, like hydrogen and carbon/oxygen, when they are contrasted with much heavier metals in the same structure.

The MOFs were synthesized in collaboration with Professor Eric Bloch’s laboratory at the University of Delaware and the activation procedures were analyzed at NIST through thermogravimetric analysis and X-ray diffraction. Brunauer-Emmett-Teller (BET) theory was utilized to interpret adsorption isotherms of nitrogen at various pressures to determine the surface areas of the MOFs. Temperature dependent adsorption profiles were analyzed to determine the heats of adsorption.

Using the high-resolution neutron diffractometer (BT-1), we have begun to determine the degree of solvation of these ‘activated’ MOFs, through structural determination; the degree of residual solvation being a factor we suspect influences adsorption characteristics. We further aim to determine the locations of the adsorbed CO₂ molecules and correlate the adsorption characteristics to the structural properties for a series of mixed-metal MOFs.

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### Omar Cavazos

**Name:** Omar Cavazos  
**Grant Number:** 70NANB17H136  
**Academic Institution:** Texas A&M University-Kingsville  
**Major:** Mechanical Engineering (Nuclear Engineering Minor)  
**Academic Standing (Sept. ’17):** Senior  
**Future Plans (School/Career):** Pursing a Graduate Degree in Mechanical Engineering  
**NIST Laboratory, Division, and Group:** NIST Center for Neutron Research (NCNR), Reactor Operations and Engineering Group  
**NIST Research Advisor:** Dagistan Sahin  
**Title of Talk:** Reactor Control Interface Design  
**Abstract:**

National Institute of Standards and Technology (NIST) has a 20 MW, heavy water moderated nuclear reactor. The control system of the National Bureau of Standards Reactor (NBSR) is being upgraded. Human Machine Interface (HMI) design is a key component of this upgrade and is important for operational performance of the NBSR reactor. Modern digital control systems and HMI mimic diagrams are being implemented. It has been noted that a well-designed HMI can reduce training time, startup or shutdown durations, and minimize operator fatigue. Research in human factors and ergonomics has been conducted to provide guidance while designing the new HMI. Therefore, Nuclear Regulatory Commission (NRC) guidance, particularly focusing on reliability, adequacy, safety, redundancy, and simplicity was followed.

SolidWorks software was used to generate a 3D model and 2D technical drawings of the proposed HMI layout. Previous drawings of the reactor control console and product manuals were used to model the control system console to scale. The new layout was designed according to industrial codes and standards. The Department of Defense Design Criteria Standard for Human Engineering (MIL-STD-1472G) was used intensively to lay out the displays and controls on the interface. The reactor operators were crucial to the design of the upgrade. Several interviews were conducted to acquire feedback for the design. After the design was finished, a human performance analysis, which describes how the system meets design criteria and design bases, was conducted. The final HMI design was printed as a poster and placed in the control room for a course of 2 weeks. This gave time for all the operators to review the final HMI design and provide final comments. Also, a mock-up of the storage pool section was set up to observe the human performance of the HMI design.
Elucidation of Insulin Structure Under Shear Using Small Angle Neutron Scattering

Abstract:
Engineered insulin analogue N-lithocholyl insulin is known to self-associate into rod-like oligomers in subcutis, from which monomeric subunits release at a slow and consistent rate at the ends. This process is well-studied in different chemical environments for its application in developing long-acting insulin treatments for patients with diabetes. However, the impact of shear stress, which occurs during insulin injection and intravascular transport, on self-assembly is still poorly understood. This study therefore seeks to investigate insulin’s structural and rheological properties under shear. Small Angle Neutron Scattering (SANS) was used to obtain structural information during application of shear in a rheometer across shear rates from 0–3500 s⁻¹. Though this range is lower than those of syringe needles and capillaries, the experiment still provides useful preliminary data for future simulations involving higher shear rates. NaCl and insulin concentrations were also varied to simulate environments in subcutis and in formulation. SANS data provide evidence of rod formations that lengthen with increasing salt concentration in solution, as expected from previous studies. The data further suggest quadratic (square pattern) ordering of these rods for a small number of samples at high salt concentrations. For all insulin samples, viscosity decreased with shear at low shear rates and increased with shear at high shear rates. However, as little to no shear-induced structural changes were apparent at the length scale probed by SANS, we determined that the insulin rheology was as related to the dynamics of the insulin rods than their structural rearrangement.

Multimode Characterization of Multiscale Structural Architectures in New MoS₂–S Composite Cathodes for High-Energy Density Li–S Batteries by Focused Ion and Electron Beam Techniques

Abstract:
Li–S batteries are of great interest as an emerging high density energy storage technology to realize ever growing demands in electrification, mobile electronics and national security. Recently, high-performance Li–S cathodes were formulated with composites comprising elemental sulfur and MoS₂, a prospective 2D layered material. It is suggested that MoS₂ can bind polysulfides (Li₂Sₓ, 1 ≤ x ≤ 8) formed as products of the electrochemical reduction of sulfur and may catalyze the polysulfide redox reactions. Binding of polysulfides is an important approach to enhance cycle lifetime of the Li–S cells by decreasing losses of the active material.

To understand the mechanisms responsible for such remarkable performance, we investigated the topography, morphology, crystallinity, and chemical compositions of the cathodes and their components at multiple scales using a combination of multimode correlated focused ion and electron beam microscopy techniques. We found that the cathodes consist of 3 mm to 15 mm α–Sₙ particles and 5 mm to 40 mm hexagonal 2H-MoS₂ flakes dispersed in a matrix of conductive carbon, which is composed of aggregated 30 nm to 60 nm amorphous particles. Ball-milled 3D MoS₂ flakes appear to have defective microstructures resulting from partially exfoliated high-aspect ratio sheets and agglomerates of crystallites with a mean size of 1 μm, different orientations and multiple defects particularly at corners of the crystallites. Structural analyses indicate that such defects could serve as potential anchoring sites. Polysulfide precipitates in cycled cathodes were often found to grow on the edges of 2H-MoS₂ crystallites, whereas on basal planes the amount of precipitates could be less, suggesting selectivity of edge versus basal sites. Our findings point to the crucial ability of MoS₂ to anchor polysulfides during cycling, elucidating the mechanisms responsible for the excellent capacity retention of the cathodes and pushing towards higher rate capability Li–S batteries.
**Title of Talk:** Phase Behavior and Structure of Microemulsions

**Abstract:**
Microemulsions are thermodynamically stable clear solutions which consist of water, oil, and amphiphile formed under very low interfacial tension. Despite numerous applications and decades of research, microemulsion phase behavior and microstructure are not fully understood. Previously, our group has found that a mixture of an extended anionic surfactant, an alkane mineral oil, and brine, in certain proportions, will form an interesting thixotropic microemulsion. In this work, the phase behavior of a similar surfactant system is investigated in combination with a variety of alkanes and as a function of brine concentration. Visual inspection is used to map the phase diagram as a function of composition. Small angle neutron scattering (SANS) is used to measure the domain size in the middle microemulsion phase of the samples. The thixotropic shear induced “gelation” response is observed only at the optimum brine concentration, where the interfacial tension is minimized. Based on the microemulsion phase diagram, samples are prepared at the optimum salt concentration and altered such that only a water phase and microemulsion phase are present (the oil phase is eliminated), and the oil:water ratio under these conditions is varied. The samples are then vortexed to determine the range of oil:water ratio where gelation is observed. Rheology is used to characterize the strength of the gel and the time scale of the thixotropy. Furthermore, rheoSANS is used to directly link the structure and rheology during the microemulsion gelation formation.

**Title of Talk:** Evaluating Combined Shear and Compression Test Methods for Impact Mitigating Materials

**Abstract:**
An important consideration in the design of any impact-resistant head equipment, such as a football helmet, is that the equipment exhibit superior performance under not only compressive stress but also shear stress. The shearing force during an impact to the head can cause serious neurological injuries by imparting sudden rotational acceleration to the skull relative to the brain, stretching or severing nervous connections in the process. Compression typically occurs simultaneously with the shearing force in such impacts; however, impact mitigating materials have previously been tested separately for their resistance against these two forces. For accuracy, test methods that combine both shear and compression forces have been developed to better characterize the coincident mechanical behaviors of materials during impact. At present, these test methods are still not well understood and need further optimization.

One such test method involves applying lateral compressive stresses to a sample test material using pressure plates and simultaneously releasing a drop mass on to the material from controlled heights to apply shear impact. Compression typically occurs simultaneously with the shearing force in such impacts; however, impact mitigating materials have previously been tested separately for their resistance against these two forces. For accuracy, test methods that combine both shear and compression forces have been developed to better characterize the coincident mechanical behaviors of materials during impact. At present, these test methods are still not well understood and need further optimization.

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### Abstract:

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is a powerful technique for the detection of chemical species on a surface while preserving their spatial distribution. With the advent of a new cluster source, 3D maps of molecules within an organic matrix can now be readily obtained. This is exciting as it offers a new way to characterize organic materials that are relevant to fields such as forensics and additive manufacturing. Examples include the analysis of fingerprints for purposes of linking an individual to a crime scene through the detection and quantification of illicit drugs, as well as for validating the quality of drug delivery films through the visualization of multilayer structures or pharmaceutical distribution that may be vital for effective drug delivery.

For this technique development, fundamental understanding of matrix effects and the instrument’s detection limit and quantification limits were tested using cocaine, buprenorphine, and naloxone. Calibration test samples were made using a piezo-driven, drop-on-demand printer that deposited the molecules on matrix-matched surfaces (cocaine on fingerprints and buprenorphine/naloxone on drug films) at surface concentrations that ranged from 5 pg to 5 ng of material per droplet, with less than 2% RSD. The spots on the surfaces were analyzed using ToF-SIMS and a calibration curve relating the signal intensity to the amount of drug deposited was produced to focus on the instrument’s limit of detection and limit of quantification. The detection of cocaine has shown a linear trend with a lower limit of 10 pg on a gold surface. Buprenorphine and Naloxone also show linear trends with r-squared values of 0.97 for masses ranging from 12 pg to 5 ng and 25 pg to 2 ng respectively. Additional testing is needed to establish lower limits of detection for cocaine on a fingerprint surface, buprenorphine, and naloxone.

### Materials and Methods:

1. **Materials**:
   - Perovskite samples were made using typical powder processing techniques.
   - The structure and phase purity of the processed samples were characterized by classical techniques such as x-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM).

2. **Instrumentation**:
   - Electron paramagnetic resonance (EPR) was used to characterize the lattice site location and valence states of the manganese ions.
   - Through the application of a magnetic field, the degeneracy of unpaired valence electrons in manganese is lifted allowing these ions to absorb quantized values of microwave energy at specific magnetic fields dependent on the location of the ion in the lattice, its local structure, and its valence. The EPR signals of manganese ions are well understood, allowing these ions to be used as probes into the perovskite structure and local defect chemistry.

3. **Techniques**:
   - Additional testing is needed to establish lower limits of detection for cocaine on a fingerprint surface, buprenorphine, and naloxone.

### Results:

- **Quantification of Drugs**
  - Oxides are important functional materials used in a variety of applications, ranging from capacitors and energy storage devices as insulators, to fuel cells and photovoltaics as conductors. One of the most important crystal structures for functional oxides is the perovskite structure. Oxygen vacancies are often the primary mobile point defects in perovskites, as opposed to electrons or electron holes. The effects of large concentrations of these charge-carrying defects can be detrimental when the material is used in insulating applications by contributing to the resistance degradation of the material, and allowing it to become conductive over time.

  - In this study, perovskite samples were made using typical powder processing techniques. The structure and phase purity of the processed samples were characterized by classical techniques such as x-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The perovskites were then intentionally doped with the paramagnetic transition metal ion manganese. Electron paramagnetic resonance (EPR) was used to characterize the lattice site location and valence states of the manganese ions. Through the application of a magnetic field, the degeneracy of unpaired valence electrons in manganese is lifted allowing these ions to absorb quantized values of microwave energy at specific magnetic fields dependent on the location of the ion in the lattice, its local structure, and its valence. The EPR signals of manganese ions are well understood, allowing these ions to be used as probes into the perovskite structure and local defect chemistry.

- **Characterization**
  - This manganese ion probe was successfully used to determine the site occupancy of co-dopant ions, such as magnesium and cerium, as well as the behavior of oxygen vacancies in the perovskite structure. Measurements were made on the materials to determine the effects these dopants have on functional properties. Moving forward, this technique could contribute to the improvement and reliability of oxide dielectric devices by significantly extending their lifetimes through dopant engineering.
**Abstract:**

The limitations of current electron microscopy data curation practices are felt whenever a scientist wishes to revisit data. A single microscopy session can generate hundreds of files. It can be a time-intensive task to determine contents of each file consisting of an image or a spectrum and the associated metadata. In some cases, an image thumbnail may be available, but an image alone usually lacks contextual information. This inevitably forces scientists to comb through files sequentially, using instrument or detector-specific proprietary software to view data and metadata. This method of data examination limits the significance of each file to a combination of the researcher’s notes or memory, OS-generated metadata (file size and time stamp), an instrument or detector-specific proprietary software to view data and metadata. This method of data examination limits the significance of each file to a combination of the researcher’s notes or memory, OS-generated metadata (file size and time stamp), and perhaps file naming convention. This is not a tractable premise for the hundreds of images for a given sample, thousands of images that may have contributed to publications, and hard drives full of project data contributed by multiple researchers over the span of a project. Ultimately, individually managed data and metadata based on project discipline, chronological order, or some other arbitrary user preference is fundamentally lacking in transparency, longevity, and reusability.

With increasing demands of open data for research produced by public funds, research needs to shift towards thoughtful data preservation and annotation. Laboratory information management system (LIMS) are often intended to manage data as soon as it is created. A LIMS platform would be an enabling component towards better adoption of FAIR (Findable, Accessible, Interoperable, Reusable) data principles. Among the many open source data coordination and curation options presently available, MML is developing a pilot based on the T2C2 4CeD curation and coordination framework for the Electron Microscopy Nexus (a shared facility within MML). For this presentation, we will share the progress we made and the lessons we learned in tackling this ambitious but essential step in modernizing electron microscopy data infrastructure.
Title of Talk: Copper Electrodeposition on a Rotating Disk Electrode: Hydrodynamic Effects on Spatial Patterning in the Presence of a Polymer-Chloride Adlayer

Abstract:
High aspect ratio trenches, referred to as through silicon vias (TSVs), are used in the microelectronics industry as interconnects for 3D stacking of integrated circuits. During fabrication of TSVs, these trenches are filled with copper through a process called bottom-up superfilling, which causes electrodeposition to be localized to the bottom of the TSVs. The physicochemical phenomena enabling this is a polymer-chloride adlayer that suppresses copper ion access to the electrode coupled to resistive losses (IR-drop) through the electrolyte solution. Essentially, the copper-seeded substrate separates into active regions (bottom of the TSV) where the adlayer is desorbed and copper deposition occurs freely and passive regions (top and side walls of the TSV) where the suppressing adlayer inhibits electrodeposition. Designing these systems requires intricate understanding of the nature of the polymer-surface complex, electrolyte solution properties (such as composition and solution resistance), and effect of potential on the active/passive kinetics of copper electrodeposition.

In this study, a rotating disk electrode (RDE) system is used to study the effect of hydrodynamics on copper pattern formation. Polymer-chloride adsorption/desorption characteristics are changed by controlling chloride and polymer concentrations, solution resistance is adjusted with the supporting electrolyte concentration (sulfuric acid), and hydrodynamics are controlled with the RDE rotation rates. The above parameters are evaluated by measuring various potentiodynamic and galvanostatic techniques and imaging copper pattern formation with optical microscopy. Optical microscopy shows that varying the RDE rotation rate while holding constant current generates copper patterns of varying striation density, indicating that hydrodynamics affects the polymer adsorption/desorption behavior. Additionally, increasing the solution resistance or decreasing current density increases striation density for a given rotation rate, which is consistent with previous studies in stagnant and rotating fluid fields. Pattern initiation appears independent of surface defects inherent to the RDE, and thus believed to be generated solely by polymer desorption. Our experimental results show that hydrodynamics can help control pattern formation and that the rate of rotation affects the density of striations, which is in opposition to previously published studies claiming pattern density is only a function of current density. Further research is needed to fully understand the desorption mechanism for the polymer-chloride complex and spatial localization of this phenomenon. Controlling the hydrodynamics in these systems may be useful to guide pattern formation for producing high-end microelectronic interconnects.

Anderson and Camley (Phys. Rev. B, 2016) have predicted that interfacial antiferromagnetic (anti-parallel) coupling of the magnetic moments in simulated core/shell nanoparticles composed of Fe and Gd may lead to large tunable variations in magnetization with temperature, not present in FeGd alloys. Guided by this theory, Fe/Gd/Fe and Gd/Fe/Gd trilayer samples of three total thicknesses (15 nm, 30 nm, 42 nm) were prepared with the atomic fractions of the most interesting simulated nanoparticles. The magnetic moment of the sample was measured as a function of temperature and applied field using a magnetometer (SQUID VSM). Over the range 100 K to 350 K under an applied magnetic field of 0.1 T, the trilayer samples showed changes in magnetization as large as 15%, compared with 4% for an Fe monolayer. In addition, several samples exhibited unusually complex behavior, with multiple local minima/maxima over the course of a magnetization versus temperature experiment. Furthermore, distinct changes in the shape of the magnetization with magnetic field measurements (square vs. S-shaped) confirm these results. To better understand what is occurring experimentally, confirmation of the crystal structures will be performed using transmission electron microscopy, as well as confirmation of the fundamental magnetic parameters for micromagnetic modeling. In conclusion, trilayer nanomaterials of Fe and Gd have been shown to provide the large changes in magnetization necessary to improve signal-to-noise for applications in magnetic nanothermometry.
**Title of Talk:** A novel chromatographic approach to characterizing monoclonal antibody aggregation kinetics

**Abstract:**

Protein drugs have revolutionized the treatment of chronic diseases, allowing for dramatic increase in quality of life for patients suffering from diseases like rheumatoid arthritis, ulcerative colitis, and Crohn’s disease. Protein therapeutics have been largely successful in recent years, with the total biologic market projected to reach $500 billion (US) in sales per year by 2024, which is equivalent to the annual GDP of Sweden. Realizing their potential, the pharmaceutical industry has taken interest in better understanding biologics. While protein-based drugs must maintain activity during manufacturing, storage, and transportation, they are particularly susceptible to chemical and physical degradation. Even under favorable storage conditions, these drugs aggregate, where multiple protein molecules assemble in an uncontrolled and undesirable fashion into large particles. The resulting aggregated therapeutic can be extremely unsafe for use and can result in negative effects, including embolisms, renal impairment, and immunogenic responses.

Understanding the kinetics behind aggregation is essential in predicting the shelf life of a therapeutic. To this end, an accelerated stress test was performed using NIST monoclonal antibody (mAb, ref. material 8671) with varying protein concentrations and elevated temperatures. The disappearance of monoclonic antibody through transformation into aggregates was monitored as a function of time using tandem asymmetric flow field flow fractionation (a type of chromatography) and multi-angle light scattering. The rate of change from monomer to aggregate was fit to a standard Arrhenius model, allowing for the prediction of the aggregation rate constant for any temperature. Knowing the rate constant, the expected shelf life of the NIST monoclonal antibody can be determined for various storage conditions. Further, these results lay the foundation for the development of a standard nanoscale protein aggregate. A standard protein aggregate will allow for characterization and comparison of protein therapeutics over the course of manufacturing, storage, transportation, and ultimately, use.

- **Name:** Jeremy Filteau
- **Academic Institution:** Worcester Polytechnic Institute
- **Major:** Chemical Engineering
- **Academic Standing:** Senior
- **Future Plans:** Pursuing a career in chemical engineering
- **NIST Laboratory, Division, and Group:** Material Measurement Laboratory, Biomolecular Measurement Division, Bioprocess Measurements Group
- **NIST Research Advisor:** Wyatt Vreeland
- **Grant Number:** 70NANB17H146
- **Title of Talk:** A novel chromatographic approach to characterizing monoclonal antibody aggregation kinetics

**Abstract:**

The composition of polymers determines their properties and performance. A cross-linking copolymer with a well-controlled composition is vital for material performance but very difficult to prepare. In general, the feeding composition of monomers is not the same as their polymers’ composition. In this work, two monomers, urethane dimethacrylate (UDMA) and triethylene glycol-divinylbenzyl ether (TEG-DVBE) were used to create composition-controlled polymers. As the monomers cure, both UDMA and TEG-DVBE decrease in concentration and a polymeric network forms. If both monomers are converted at equal rates, the reaction is described as composition controlled. The primary goal of my summer project is to build an instrument monitoring the composition of UDMA/TEG-DVBE during photo-polymerization in real-time and evaluate the kinetics of the composition controlled copolymerization. The second goal is to establish a correlation of polymer composition with their mechanical performance. Mixtures of equimolar UDMA and TEG-DVBE were activated by photoinitiator camphorquinone and amine for blue light induced photo-polymerization. Raman spectroscopy and near infrared spectroscopy were used to monitor the composition of polymers and the progress of the polymerization/curing of monomers. Simultaneously, this instrument can assess the stress development during polymerization through a combined tensometer. The data obtained from here were used to determine the degree of conversion (DC) of each monomer, which was further applied to assess whether the polymerization is composition controlled or composition shifted, and how the composition change affects mechanical performance in terms of polymerization stress and Knoop hardness. High DC at approximately 80 % were achieved with exposure light intensities between 20 mW/cm² and 100 mW/cm² and only composition controlled polymers were obtained with equimolar feeding composition. In conclusion, the instrument was successfully built and applied to evaluate the composition during photo-polymerization at different light intensities. Future work involves determining composition and polymerization stress simultaneously, evaluating mechanical properties of the cured samples, understanding the mechanism of composition controlled photo-polymerization.

- **Name:** Ethan Finlay
- **Academic Institution:** Appalachian State University
- **Major:** Physics and Chemistry
- **Academic Standing:** Senior
- **Future Plans:** Get a M.D. or M.D./Ph.D. and become an Endocrinologist.
- **NIST Laboratory, Division, and Group:** Materials Measurement Laboratory, Biosystems and Biomaterials Division, Biomaterials Group
- **NIST Research Advisor:** Jirun Sun
- **Grant Number:** 70NANB17H064
- **Title of Talk:** Composition Controlled Photo-Copolymerization: Evaluation, Kinetics and Properties
**Title of Talk:** Raman and THz Raman Spectroscopy for Forensic application of illicit narcotics and explosives.

**Abstract:**

The struggle against domestic and international terrorism has become a crucial challenge for the safety of United States citizens. An important aspect of this task is the development of sensitive, low-cost technologies that can be deployed in the field for the detection of explosives. Among the available detection technologies, Raman Spectroscopy has recently gained increasing interest for possible application in rapid screening for explosives at security checkpoints and as a tool for presumptive drug testing in forensic laboratories. The focus of our research was to evaluate the use of Raman and THz Raman spectroscopy for the detection of explosive compounds and to measure the sensitivity of a commercial Raman microscope instrument for trace optical analysis. The samples of explosives were analyzed to obtain Raman spectra from each analyte and develop the Raman and THz Raman database. This database was created to aid in the development of detection algorithms for trace contraband screening.
SURF Student Colloquium  
NIST – Gaithersburg, MD  
August 1-3, 2017

Name: Ray Shimmi Geretsa  
Grant Number: 70NANB17H085

Academic Institution: Montgomery College  
Major: Aerospace engineering

Academic Standing: University of Maryland College Park, 3rd-year Undergraduate

Future Plans: Planning on going to graduate school and focus on space debris removal

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Material Science and Engineering Division, Functional Polymers Group

NIST Research Advisor: Edwin P. Chan

Title of Talk: The Nature of Gelatin Fracture

Abstract:

Gelatin is widely used in the manufacturing of soft and hard-shell capsules used by the pharmaceutical industry. One of the ways in which the drug is released is via rupture, i.e. the fracture, of the gelatin capsule after being ingested. Quantifying the resistance to fracture, such as the energy release rate ($G_c$), of gelatin can be effective in designing a drug delivery system capable of delivering a drug over an extended period of time at a controlled rate. We study this fracture behavior using cavitation rheology (CR), which is a mechanical testing technique that quantifies $G_c$ by measuring the critical pressure required to nucleate a bubble to mimic a fracture event.

Specifically, we use CR to measure the $G_c$ of gelatin formulations as a function of gelatin volume fraction ($\varphi$) with respect to water. We find that the $G_c$ scales proportionally with $\varphi$ up to a critical $\varphi$ and then drops as $\varphi$ continues to increase. More importantly, we find that this scaling is related to the size-scale and distributions in the mesh size of the gelatin network as measured by small-angle neutron scattering. The implication of this study is that the fracture properties of gelatin can be controlled by the network structure of gelatin via $\varphi$.  

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SURF Student Colloquium  
NIST – Gaithersburg, MD  
August 1-3, 2017

Name: Brady Garringer  
Grant Number: 70NANB17H131

Academic Institution: Boise State University  
Major: Materials Science and Engineering

Academic Standing: Junior

Future Plans: Pursue a career in aeronautics or computational materials science

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group

NIST Research Advisor: Debra Audus

Title of Talk: Free Energy of Coacervate Core Micelles

Abstract:

When oppositely charged polymers are dissolved in water, they can phase separate into a polymer rich phase, known as a complex coacervate, and an aqueous phase with very low polymer concentrations. If neutral, hydrophilic polymers are covalently bonded to each of the charged polymers to form diblock copolymers, bulk phase separation will not occur; instead, the coulombic attraction of the oppositely charged blocks combined with propensity of the hydrophilic, neutral blocks to stay in water will cause the copolymers to arrange in a spheroid configuration with the charged blocks packed in the core of the micelle and the neutral blocks protruding from the core, forming the corona.

As these coacervate core micelles have hydrophilic cores, these micelles have theorized application in targeted, hydrophilic drug delivery. For this application, knowing the size of the micelles in critical for determining the quantity of drug that can be stored in the core. Thus, the goal is to establish micelle size as a function of concentration, which can be derived from the relationship between the free energy of a micelle and number of polymers in a micelle, also known as the aggregation number. To compute the free energy, one pair of copolymers, each with oppositely charged charged blocks, is pulled out of the micelle and held at a set distance away from the center of mass of the core using a technique called umbrella sampling. Umbrella sampling involves forcing the system into states that are unlikely to be found naturally in order to access relevant, but rare events. The resultant attractive force that is pulling the pair back toward the micelle can be used to compute the free energy as a function of distance, also known as the potential of mean force, and associated error using the weighted histogram analysis method. Using the potential of mean force, the free energy change and error can be calculated using various statistical techniques. This can then be used to compute the aggregation number, and thus the micelle size, as a function of concentration.
Name: Andrew Gayle  
Grant Number: 70NANB17H072  
Academic Institution: Duke University  
Major: Mechanical Engineering  

Academic Standing: Sophomore  
(School/Career): Pursue a doctorate and continue a career in industry that involves computational biology or chemistry.  
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Biomolecular Measurement Division, Mass Spectrometry Data Center Group  
NIST Research Advisor: Xiaoyu (Sara) Yang  
Title of Talk: Enhancing the Process for More Accurate Compound Identification in the NIST Tandem Mass Spectral Library  

Abstract:  
The NIST Tandem Mass Spectral Library with comprehensive and high quality reference mass spectra has been widely used in the identification of compounds through the fragmentation of their ions generated by electrospray ionization mass spectrometers in biomedical studies. It is integral that the chemical information that is used in this library be accurate for subsequent valid identification results. However, to manually inspect thousands of compounds and check chemical information (CI) errors would be highly time-consuming and nearly impossible. The objective of this project is to develop a computer program in C++ that can quickly proofread the chemical information to ensure their accuracy for the library.  

Two databases (metabolite and peptide), each of which stored a range of 2,500 to 17,000 different chemical compounds, each compound containing 15 to 17 features which are pertinent to its identity (primary name, chemical registry number (CAS), formula, other names, etc.) were analyzed. A computer program, _CI_checker_, was developed to perform the following tasks: (1) it searched for primary name matches between compounds of both databases; (2) based on the matched primary names of the compounds, it analyzed those matches to ensure chemical accuracy with corresponding matching CAS, formula, other names, and related CAS; (3) if a pair of compounds did not match in any of those features, or a compound contained any other type of error (e.g., duplicate, mismatch, missing entries, types) they were outputted to an excel file, name specified by users, indicating the error type.  

All the features of the compounds in each database were saved as structs, all contained in a string indexed map specific to compound type (e.g. metabolite or peptide). By using map string indexing as a container for the compounds, the program run time was optimized to ~1.5 minutes. This program found that 300 compounds had their CAS numbers missing; 4 compounds had names duplicated in both the primary name and synonym within the synonym itself; 200 compounds did not have their CAS numbers saved in a standardized format; and various other errors that would have otherwise taken too long and been difficult to have been caught manually.  

_CI_checker_ program was tested with the chemical databases for the NIST Tandem Mass Spectral Library. It was also made to be user-friendly for chemists and efficient at analyzing the myriad amount of chemical information.
Abstract:

Materials for gas and vapor sorption find uses in many branches of science, perhaps most notably environmental applications including gas and vapor purification, capture, and storage. For example, water vapor can interfere with carbon dioxide capture from the atmosphere, so it is crucial to understand how vapors behave and what their adsorptive properties are. A useful way to analyze the vapor sorption capability of a material is to look at its vapor sorption isotherm, which plots its vapor uptake as a function of the relative pressure of the vapor, or relative humidity in the case of water vapor. To work towards further development in this field, there is a need for more consistent standards and procedures to measure the properties of these materials and to create more accurate and reproducible isotherms. For this to be possible, a thorough understanding of the instrumentation used to create the isotherm is necessary. This project looks at water and ethanol vapor sorption isotherms of two adsorbents to determine whether the temperature of the solvent reservoir has an impact on resulting isotherms. MML’s Facility for Adsorbent Characterization and Testing (FACT) Lab uses a vapor sorption analyzer, on which the temperatures of both the sample chamber containing a material that uptakes vapor and the reservoir containing the solvent can be controlled. The instrument can only reach a maximum sample chamber temperature of 150 °C, several adsorbents are available to the FACT lab were tested via thermogravimetric analysis to determine their activation temperatures. It was found that MIL-53 and ZIF-8, both of which can be activated below 150 °C, were best suited for analysis in the vapor sorption isotherm. Three water sorption isotherms at 25 °C at different reservoir temperatures (30 °C, 35 °C, and 40 °C) were produced for MIL-53. Comparison of the water sorption isotherms suggests that reservoir temperature has no effect on vapor uptake of these compounds. This was expected because even though the reservoir temperature affects the humidity of the sample chamber, a humidity sensor controls the exact humidity of the sample chamber to construct the isotherm. In contrast, there is no sensor in the instrument for ethanol and other organic solvents. In the coming weeks, ethanol sorption isotherms will be constructed with ZIF-8 at the same reservoir temperatures as the water isotherms to determine if this difference will impact the ethanol isotherms.
Molecular simulations performed at low temperatures are often significantly more computationally expensive than those at higher temperatures due to the increased difficulty of sampling configurational space. Recently, Mahynski et al. proposed a method to predict thermodynamic properties of fluids at low temperatures using only simulation data collected at high temperatures. Here, we have extended this method to demonstrate that this "histogram extrapolation" approach can also be employed to predict low-temperature structural properties.

In order to show the broad capabilities of this method, we performed Monte Carlo and molecular dynamics simulations for several coarse-grained molecular systems which exhibit a variety of different thermodynamic behaviors. We demonstrate how to extrapolate the radial distribution function for both single and multi-component systems; when appropriately combined, we illustrate how these distributions may be known over essentially the entire phase space for a fluid from only a small number of simulations, even when bulk phase separation occurs. We then turn our attention to self-assembling systems. We demonstrate how this extrapolation technique may be used to accurately predict the coil-globule transition of a 5-bead homopolymer by predicting the polymer's radius of gyration as a function of temperature. Another important quantity of interest for self-assembling systems is the concentration at which the particles first begin to aggregate, known as the "critical micelle concentration." We show two ways this extrapolation approach may be used to predict the critical micelle concentration: one by predicting the cluster size distribution, and another by predicting the thermodynamic pressure as a function of decreasing temperature.

Thus, this extrapolation approach can significantly improve the efficiency of computer simulations aimed at measuring structural quantities of molecular systems, and further enables the prediction of properties at temperatures that are too low to easily simulate directly.
### Nathaniel Kaneshige

**Name:** Nathaniel Kaneshige  
**Academic Institution:** University of Hawaii at Mānoa  
**Major:** Physics and Math  
**Grant Number:** 70NANB17H122

<table>
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<td>NIST Laboratory, Division, and Group:</td>
<td>NIST Center for Neutron Research, Research Facilities Operations Group</td>
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<tr>
<td>NIST Research Advisor:</td>
<td>Dr. Nick Maliszewskyj and Kevin Pritchard</td>
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<tr>
<td>Title of Talk:</td>
<td>6LiF:ZnS(Ag) Neutron Detector and Data Acquisition/Processing System Development</td>
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The Chromatic Analysis Neutron Diffractometer or Reflectometer (CANDOR) is a new instrument under development at the NIST Center for Neutron Research (NCNR) that will use scattering by a broad energy spectrum of neutrons to investigate the structures of materials. The triggering, discrimination, and acquisition of neutrons from a broad energy spectrum over a range of scattering and reflecting angles brings unprecedented design challenges. As well-established 3He neutron detectors would not meet the form factor requirements of CANDOR, it was necessary to develop an ultrathin neutron detector using 6LiF:ZnS(Ag) plastic scintillator coupled to wavelength shifting fibers leading to a Silicon Photomultiplier (SiPM) for readout. The signal from the SiPMs must then be processed using fast electronics to discriminate neutron capture events from other event types. At this stage, we have a highly efficient, extremely thin, neutron detector whose performance is on par with traditional 3He gas-filled tubes at a fraction of the price.

The CANDOR data acquisition (DAQ) system includes waveform digitizers, which use digital signal processing (DSP) techniques to accurately identify neutron events. For this project the neutron detection and data acquisition/processing systems were characterized and evaluated for use in the CANDOR instrument as well as for other applications.

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### Emmie Knobloch

**Name:** Emmie Knobloch  
**Academic Institution:** Smith College  
**Major:** Biochemistry  
**Grant Number:** 70NANB17H122

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<tr>
<th>Future Plans (School/Career):</th>
<th>NIH Postbaccalaureate CRTA Fellow</th>
<th>Graduate school, seeking a PhD in molecular biology or biomolecular engineering</th>
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<td>NIST Research Advisor:</td>
<td>Erica Stein</td>
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<tr>
<td>Title of Talk:</td>
<td>Assessing CD4 Receptor Expression in Jurkat Cells</td>
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**Abstract:**

T cells are a class of immune cells that play an important role in several aspects of adaptive immunity. As such, their study is crucial to an in-depth understanding of the function of the immune system. Jurkat cells are an immortalized line of human T cells that are frequently used to study various aspects of T cells, including cell signaling, T cell leukemia, and chemokine receptor expression. They are also used in bioassays that test the potency of drugs in development.

Jurkat cells are known to express low levels of CD4 receptors, a characteristic of T helper cells. However, it has also been observed anecdotally that CD4 expression levels vary and tend to decrease as passage number increases. It is important to be able to characterize the properties of a cell line so commonly used in research and manufacturing, and how they change over time. This will enable us to more fully understand how Jurkat cells simulate the function of our native immune cells.

This project aims to determine how levels of CD4 receptor expression in Jurkat cells vary with passage number and cell density by analyzing cultures over time using flow cytometry. Samples from each culture are stained using fluorescent antibodies that will bind to CD4 receptors, yielding a fluorescence measurement that can be translated into antibodies bound per cell (ABC). Changes in ABC are indicative of changes in actual CD4 expression, and will thus provide information about how CD4 expression levels in Jurkat cells vary under different conditions.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: David Lech
Grant Number: 70NANB17H146
Academic Institution: Worcester Polytechnic Institute (WPI)
Major: Chemical Engineering
Academic Standing (Sept. '17): Junior
Future Plans (School/Career): Graduate school
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Material Science and Engineering Division, Polymers Processing Group
NIST Research Advisor: Jonathan Seppala
Title of Talk: 3D printing of polymers: It’s all about the interface

Abstract:

Material extrusion is a method of additive manufacturing (AM) that heats a material to a malleable state and deposits it through a nozzle layer-by-layer to construct a desired part. AM is used in many industries requiring complex parts that would otherwise be expensive and difficult to manufacture. However, like many AM methods, material extrusion produces parts that are generally weaker than traditional manufacturing methods, a problem for industries that need parts to undergo constant wear and tear. Due to its layer-by-layer construction, this weakness can be sourced to the welds formed between each layer. In this work, the process-performance relationship of material extruded polycarbonate is measured and compared over a range of printing parameters. Infrared (IR) imaging was used to observe the material extrusion process and to determine the temperature profile during prints while the weld tear energy was measured by mode III fracture. Weld times were calculated from the temperature profiles and a relationship between weld time and tear energy is compared. Understanding inter-layer mechanics and the role of printing parameters on weld strength will bring us closer to optimizing overall part strength.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Dmitry Leontyev
Grant Number: 70NANB17H164
Academic Institution: University of Maryland, College Park
Major: Chemistry
Academic Standing (Sept. '17): Junior
Future Plans (School/Career): Currently set on a Pharmaceutical Science PhD program offered at UMD, School of Pharmacy. But am also considering other potential PhD programs related to chemistry.
NIST Laboratory, Division, and Group: Material Measurement Laboratory (MML); Materials Measurement Science Division (MMSD); Surface and Trace Chemical Analysis Group (643.05)
NIST Research Advisor: Edward Sisco
Title of Talk: Optimization of mini-DART-MS for the Detection of Smokeless Powder Residues

Abstract:

Over the last few decades there has been a rise in the use of home-made explosives for acts of terrorism, many of which have utilized smokeless powder. While attacks have exploited this material, there is not a large amount of research surrounding whether trace explosive detection technologies can detect them. The goal of this project was to optimize the parameters of a mini DART-MS (Direct Analysis in Real Time-Mass Spectrometry) system for the detection of common chemicals found in smokeless powder residues and perform several additional studies on analytical metrics.

Smokeless powder, an environmentally friendly alternative to black powder, is a mixture of chemicals including propellants, detergents, stabilizers and other additives. Traditionally, analysis of smokeless powder, or its residue, has been completed using GC/MS (Gas Chromatography Mass Spectrometry) or LC/MS (Liquid Chromatography Mass Spectrometry). While these methods can provide a wealth of information, they are accompanied by considerable wait times and lengthy sample preparation. DART-MS, an emerging trace detection technology, overcomes these hurdles by allowing analysis of samples with minimal to no sample preparation in a matter of seconds.

This project utilized a mini DART-MS system to develop an optimized method for the detection of chemicals commonly found in smokeless powders. Once established, additional studies on other analytical metrics were performed and included identifying limits of detection (LODs), understanding the repeatability and reproducibility of the system, evaluating the effects of competitive ionization, and comparing the analysis of pure compounds to actual powders. Initial work has focused on the detection of ethyl centralite, diphenylamine, dibutyl phthalate, nitroglycerin, and n-nitrosodiphenylamine. LODs have been found to be in the range of hundreds of picograms per swipe and binary mixture studies show minimal competitive ionization effects. Given these results, DART-MS shows promise in the rapid detection of smokeless powder signatures.
Kevin Liu

Academic Institution: Princeton University
Major: Chemical and Biological Engineering

Academic Standing (Sept. '17): Sophomore
Future Plans (School/Career): Graduate school for engineering
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group
NIST Research Advisor: Steven Hudson
Title of Talk: Measuring Local Shear Stresses in Wormlike Micelle Flow

Abstract:
Simple liquids respond proportionally to stress, while complex fluids do not. Complex fluids can moreover exhibit non-uniform responses to stress, as was recently demonstrated with soap solutions like shampoo. These solutions comprise long wormlike aggregates or micelles of soap molecules that self-assemble. Wormlike micelle solutions can form jets of high velocity bounded by slower-moving flow when an applied stress stretches and partially breaks the micelles. We use a simple model that predicts non-uniformities in the stress of the flow to explain this unusual flow of wormlike micelles.

To test this model, we use traction force microscopy to quantify the local stresses in the flow. A flow channel was constructed such that one surface consisted of a soft, elastic gel embedded with fluorescent markers. The fluorescent marker displacement provides information on both the direction and magnitude of the local stresses. Non-interfering fluorescent markers were also added to the fluid to track the flow throughout the channel via particle image velocimetry. We find that the higher velocity in the jet corresponds to lower shear stresses and conversely, lower velocity in the slower-moving regions corresponds to higher shear stresses.

Laura Lucas

Academic Institution: The Catholic University of America
Major: Chemistry

Academic Standing (Sept. '17): Senior
Future Plans (School/Career): Attend graduate school to pursue a PhD in chemistry
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Biomolecular Measurement Division, Biomolecular Structure and Function Group
NIST Research Advisor: Ella Mihailescu
Title of Talk: Effects of Membrane Active Peptides on the Organization of Cholesterol in Lipid Bilayers

Abstract:
Phospholipid bilayer membranes contain what are known as rafts, which are areas of cholesterol-rich domains that float around in the membrane. The function of these rafts is to aide in many cellular processes. We studied the effects of various peptides on the organization of these cholesterol rafts, as well as the overall distribution of cholesterol in model membranes by using structural and thermodynamic methods. One of the peptides used is a five amino acid sequence at the end of the pretransmembrane domain of gp41, the protein found in the envelope of HIV that is responsible for the fusion of the viral and host membranes. The other peptide that was used is Piscidin 1, which is from a family of antimicrobial peptides with anticancer properties that come from fish. We used x-ray diffraction and differential scanning calorimetry in order to study the interaction of cholesterol and these peptides in a phospholipid bilayer. X-ray diffraction was used to examine the structure of cholesterol-containing bilayers before and after adding one of the peptides. Differential scanning calorimetry was used to construct phase diagrams to analyze how each of the peptides affected the temperature of the phase transitions of the components in the bilayer. The results indicate that both the gp41 peptide and Piscidin 1 influence the segregation of cholesterol in the bilayer, but by different mechanisms. The gp41 peptide tends to cluster the cholesterol together into domains, forming cholesterol crystals in the bilayer, while Piscidin 1 prefers to separate from cholesterol and partition into the fluid phase. Overall, this study points to the importance of cholesterol and membrane reorganization in microbial invasion.
Title of Talk: First Principles Study of the Energetic Ordering and Phase Stability of Bulk and Nanostructured TiO$_2$

Abstract:

Titania (TiO$_2$) has been widely used for applications from UV protection to the decomposition of various pollutants. For future clean energy, titania has been investigated for its potential photovoltaic applications for solar panels in the conversion of solar energy into electrical energy. This material is of interest due to its tunable electronic properties, low cost, stability and non-toxic nature. In nature, titania can exist as the minerals rutile, anatase, and brookite, as well as the high-pressure phase columbite. Experimental research has determined the relative enthalpy of these titania polymorphs. A vast number of first principles studies, using density functional theory (DFT), have attempted to reproduce experimental data and have failed to reproduce the relative enthalpies. Growing interest in nanostructured titania for photovoltaic applications has spurred investigations into bulk titania to create accurate models at the nanoscale. It is essential to accurately predict structural details for a theoretical assessment of structure-property relationships.

In this study, the four titania polymorphs were investigated through DFT calculations using the Vienna ab-initio simulation package (VASP). Varying exchange-correlation (XC) functionals for the generalized gradient approximation (GGA), meta-GGA and Van der Waals (VDW) approximations were explored. Furthermore, Hubbard corrections were used to account for d electron interactions of titanium atoms. Using DFT calculations it was demonstrated that sufficiently accurate values of the polymorph's energetic ordering could be achieved using van der Waals and Hubbard corrected DFT at the GGA level. Additionally, the Hennig group genetic algorithm for structure and phase prediction-Python (GASP-Python) was run in parallel on a computer cluster using VASP. This genetic algorithm treats atomic configurations as "organisms", where the "most fit" (lowest energy) are selected, crossed and mutated to predict the optimal structure[s]. Results from GASP calculations produced interesting structures for both bulk and nanowire titania.
Quantitative Analysis on the Effects of Noise and Gaussian Blur on Hyperspectral Unmixing Algorithms

Abstract:

Hyperspectral imaging (HSI) techniques capture hundreds to thousands of colors per pixel, which may be used to ascertain the materials present within each pixel. HSI methods have been utilized in geosensing and astronomy for decades, but recently there has been significant interest in its application to biological and medical imaging. A particular challenge for HSI is the determination of the spectral signatures of pure materials as each pixel may contain a mixture of materials. Many algorithms have been developed for "endmember extraction" (also known as "spectral unmixing") for this task and to determine the relative abundances of the materials at each pixel.

Many of these algorithms assume that the spectra at each pixel can be expressed as a linear, additive combination of the individual spectra of the materials. Many algorithms also exploit the simplistic geometries of the mixed spectral vectors to unmix the hyperspectral images, where the vertices, called endmembers, are the pure spectra of the materials.

The following study quantitatively compares many commonly used hyperspectral unmixing algorithms, including VCA, N-FINDR, MVC-NMF, and SSAL, in the presence of varying amounts of noise and Gaussian blur using both simulated and real data sets. Specifically, I created a MATLAB code to execute the algorithms and compare their results to ground-truth data. The computation time, root mean square error of the abundance maps & spectra, spectral angle distance, spectral correlation measure, and spectral information divergence are used as metrics to compare the algorithms.

This work is concerned with identifying the range of standard deviations of the Gaussian distribution that the algorithms can accurately operate in, as well as comparing their performance in the presence of noise. Other considerations include the sensitivity of MVC-NMF & SSAL to initialization, the effects of dimensionality reduction on VCA & N-FINDR, and the computational cost of the algorithms.

Each of the algorithms have advantages and disadvantages; careful selection of these algorithms can lead to significantly more accurate results when compared to ground-truth data. The comparison of modern hyperspectral unmixing algorithms should increase the pace at which the algorithms can be implemented for biological and medical imaging.
One of the data analysis tools utilized by researchers at the NCNR is called bumps, a program written for curve fitting data and performing uncertainty analysis. Depending on the data sets and chosen optimizers, bumps can be computationally expensive to run. Since it was built to take advantage of parallel processing, its performance would benefit greatly from running in a high-performance environment. To that end we present work on a web service which allows for the scheduling and running of bumps jobs on remote work servers. This allows bumps to take advantage of the parallelism capabilities typically found in these servers, without requiring the end-user to set up a personal work environment.

The motivation behind the service was to provide an approachable interface for running performance-heavy computations with minimal setup. The web service is written in Python and provides a client-server interface for computations with minimal setup. The web service is written in Python and provides a client-server interface for well as a web page where the commands can be parsed and executed from traditional web forms and where job progress can be monitored. The implementation does not require administrators to manage user accounts, and it provides a Docker container as a convenient mechanism for deploying the necessary infrastructure onto the servers.

Title of Talk: Comparative LC-MS/MS Analysis of Bacterial Metabolomic Profiles: P. aeruginosa and S. aureus in Co-culture

Abstract: Pseudomonas aeruginosa and Staphylococcus aureus are both potent pathogens that frequently coexist in and confound the same physiological environments in various human disease states. P. aeruginosa can cause fatal opportunistic infections in immunocompromised individuals, and S. aureus causes severe skin, soft tissue, bloodstream, bone, and joint infections. Although both microbes are highly virulent independently, evidence suggests that when found together in co-culture, the subsequent infection results in worse patient outcomes. In certain types of infections, this is a result of P. aeruginosa antagonizing S. aureus, while in others it is due to a potentially symbiotic relationship stemming from both species’ propensity for antimicrobial resistance and biofilm formation. This co-culture is especially pertinent to chronic lung infections that constitute the principal cause of mortality in cystic fibrosis (CF) patients. These species are also the most commonly associated pathogens in wound infections, with co-infections exhibiting increased virulence when compared to that of either species in monoculture. Despite the prevalence of this bacterial system in human disease, the regulatory genetic and biochemical mechanisms involved in this complex interspecies interaction are not yet understood.

This project aims to analyze the intracellular and extracellular global metabolite profiles of P. aeruginosa, S. aureus, and their co-culture to characterize interactions between the two organisms through changes in their metabolic pathways. In our initial investigation of this polymicrobial community, we sought to promote the growth of cultures with properties most similar to those found in a CF lung infection. To achieve this, bacteria were cultured in artificial sputum medium (ASM), which has been shown to offer conditions of higher clinical relevance than traditional in vitro growth media. To study these cultures, we integrated and optimized protocols for microbial culture sampling, quantification, quenching, and metabolite extraction for analysis by liquid chromatography tandem-mass spectrometry (LC-MS/MS). Principal component analysis of preliminary data shows that differences among the metabolite profiles of P. aeruginosa, S. aureus, and the co-culture are statistically significant. It has also been found that the three samples have a number of compounds in common, and present in varying quantities among samples, suggesting up- and down-regulation of certain pathways in these species when in co-culture.

The methods developed herein contribute to efforts at NIST to develop and characterize reproducible, clinically relevant in vitro model systems for polymicrobial communities. The data compiled in this study will serve in the construction of a comprehensive reference metabolic pathway for this bacterial co-culture system, the use of which will lead to improved understanding of its role in disease, allowing for identification of novel drug targets in both species and the subsequent development of improved therapeutic agents.
**Name:** Daniel Ng  
**Grant Number:** 70NANB17H088  
**Academic Institution:** Northwestern University  
**Major:** Materials Science and Engineering  
**Academic Standing (Sept. '17):** Junior  
**Future Plans (School/Career):** BS/MS program in materials science, research and development in industry  
**NIST Laboratory, Division, and Group:** Material Measurement Laboratory, Materials Science and Engineering Division, Mechanical Performance Group  
**NIST Research Advisor:** Mark Stoudt  
**Title of Talk:** 3D Printed Pandemonium: Understanding Phase Transformations in Additively Manufactured Inconel 625  

**Abstract:**  
Additive manufacturing (AM) is a quickly growing field with promising industrial applications for fabrication of mechanical parts, and an increasing number of materials are under investigation for their feasibility in the AM process. One such material, Inconel 625 (IN625), is a nickel-based superalloy with applications in marine, nuclear, and aerospace industries due to its mechanical stability at high temperatures, as well as resistance to corrosion and oxidation. For industrial purposes, residual stress introduced during the AM process must be relieved through post-build heat treatments. However, current manufacturer-recommended heat treatments based on wrought IN625 cause precipitation of various phases in AM IN625, some of which adversely affect the toughness of the material. A lack of understanding of AM material's complicated microstructure and transformation kinetics thus leads to unpredictable mechanical behavior.  
In this investigation, heat treatments were performed on AM IN625 samples in the temperature range of 923 K to 1223 K for durations between 0.5 h and 168 h. X-ray diffraction, scanning electron microscopy, and energy dispersive spectroscopy were used to characterize microstructure and identify the acicular delta phase, and the phase fraction of delta phase in each sample was determined through a combination of computational and manual methods. The data was then compiled to generate a time-temperature-transformation diagram, which allows for optimization of the heat treatment process so that AM IN625 may be reliably used in industrial applications.
Abstract:

Immunoglobulin G (IgG) is the major type of antibody with a large Y-shape that circulates in human blood. When the human body is invaded by foreign substances, the IgGs will first attach the two upper parts of their Y-shape to pathogens to isolate them. Then these antibodies recruit other cells to initiate elimination process via subsequent interaction of their glycosylated Fc regions, which are the lower portions of the Y-shape, with transmembrane receptors such as FcγRs, of the effector host cells. Recent data have shown that glycan composition has a significant effect on antibody binding affinity to the FcγRs, and thus the efficiency of the defense mechanisms.

This project focused on NISTmAb, a reference human IgG1 monoclonal antibody produced from cell culture of identical cells that presents a precise glycosylation profile. Using highly specific endo and exo-glycosidases (Endo-S and α1,2,3,4,6 Fucosidase) in combination with glycosyltransferases (Galacto-transferase and Sialyl-transferase) we individually modified each NISTmAb glycoform in a controlled way to create glycan structures of interest. The products, which were intact NISTmAbs with desired glycan structures, were purified using Protein A affinity chromatography and detected by sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE).

In the future, isothermal titration calorimetry will be performed to determine thermodynamic parameters (binding affinity $K_d$) between the NISTmAb glycoforms and the FcγR receptors in solution. The NISTmAb-FcγR complexes that demonstrate measurable binding affinity will be incubated in deuterated water to facilitate exchange between deuterium and hydrogen of the backbone amides. Hydrogen deuterium exchange mass spectrometry (HDX-MS) will be applied to determine dynamic and conformational changes on those complexes. Based on the results and previous knowledge about IgGs, scientists can further manipulate antibody structure-function relationships to target specific diseases.

In the case of colloidal mixtures of self-assembling particles, it is often desirable to tune interactions between particles of different types to obtain specific crystal structures. These structures must be precisely ordered to be useful for optical applications such as band-gap materials. Crystallization in such systems takes place at finite temperature and atmospheric pressure, which unfortunately leads to the generation of many different polymorphs. There currently exists no rigorous technique to determine which polymorphs might form in a given system, so free energy calculations are performed on candidates drawn from libraries of known structures. Unfortunately, such “blind” searches, even through small fractions of libraries, are prohibitively expensive.

In this project, we propose a method for generating trial crystal structures and determining the most stable structures in a set based on potential energy calculations alone. It can be used to rapidly propose a small collection of structures for further, more complex processing, including free energy analysis. We have created a Python implementation of this method for two-dimensional (2D) crystals. To create a diverse set of structures, we tile a domain with randomly generated, but regularly ordered, configurations of particles using the 17 different wallpaper groups in 2D space. The basin-hopping algorithm is then applied to optimize these initial guesses and minimize their energies. We have tested the method based on literature results (molecular dynamics and Monte Carlo) for binary systems using modified Lennard-Jones-like interactions, and have found it able to reproduce them reliably at reduced computational expense. It can be extended to much more complex systems, including in theory, three-dimensional lattices.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Benjamin Dariush Rahimi
Grant Number: 70NANB17H094

Academic Institution: Catholic University of America
Major: Biomedical Engineering

Academic Standing (Sept. ’17): Graduate Student

Future Plans (School/Career): Attending graduate school at Catholic University of America. Pursuing a career in dentistry.

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Biomolecular Measurement Division, ADA Foundation-Volpe Research Center

NST Research Advisor: Diane Bieniek, PhD and Drago Skrlec, PhD

Title of Talk: Biocompatibility of Novel Antimicrobial and Remineralizing Composites for Class V Restorations.

Abstract:

DNA biosensors are an area of active research and development for targeted application in areas such as forensics and medical diagnostics. A common approach involves the use of a mixed monolayer of probe DNA and an alkylthiol on a gold substrate to measure hybridization with target DNA from solution. Additional information about duplex stability and nucleotide sequence can be obtained by modulating the duplex DNA electrochemically via the application of a sufficiently negative electrode potential. The effect of electric fields on surface-bound DNA is of great interest for understanding the hybridization and melting mechanisms of surface-bound DNA and optimizing the resulting signals. Although a complete understanding of the effect of the electric field on DNA is not yet known, studies have shown that applying a positive or negative potential can promote or inhibit DNA hybridization and can be used to control the orientation of the DNA on the surface.

In this work, the fabrication of a DNA biosensing substrate for the investigation of electric fields on DNA is presented. The dual-electrode substrate was fabricated on anodic aluminum oxide (AAO) using physical vapor deposition. An adhesion layer of 5 nm titanium, followed by 20 nm of gold was deposited on one side of the AAO. Subsequently, 5 nm titanium, followed by 20 nm of platinum was deposited on the opposite side of the AAO substrate. The films were characterized using a field emission scanning electron microscope to ensure pore size and metallic monolayers are uniform. A mixed monolayer of probe DNA and alkylthiol was assembled on the gold layer. Subsequent hybridization of a methylene blue-labeled target DNA strand results in a measurable electrochemical signal. An electric field was generated by applying a potential to the platinum electrode while the potential at the DNA-modified gold electrode was kept at open circuit potential. By monitoring the methylene blue signal at the gold electrode, the effect of electric field on DNA stability was investigated while avoiding the possibility of thiol desorption.

Objective: This study assessed the cytotoxic potential of resin components (i.e., antimicrobial and cationic QA-MA, bis(2-methacryloyloxyethyl) dimethylammonium bromide (IDMA) and urethane dimethacrylate (UDMA)) and their degradation products by using mouse subcutaneous fibroblasts (CCl1) as the standard cell line in conjunction with immortalized human cell lines such as gingival keratinocytes (Gie-NO3B11) and gingival fibroblasts (HGF-hTERT). Cell viability and metabolic activity were measured after exposure to IDMA and UDMA. Measuring these parameters will help us further understand the effects of leachable monomers at the cellular level and, in turn, will help to improve the standard of dental healthcare. Methods: The direct contact test was performed per ISO 10993-5. Briefly, HGF-hTERT, Gie-NO3B11, and CCL1 cell lines were exposed to two-fold serial dilutions of IDMA (1.6 μmol) and UDMA (1.5 mM) and their degradation products (i.e., methacrylic acid and methyl/methacrylate). After 24 and 72 h exposure, cells were assessed for viability and metabolic activity. Findings: Cytotoxic potential of acrylates can differ between cell types, thus accentuating the importance of employing biologically relevant cells in biocompatibility assessments. Data suggest that some methacrylates exhibit a greater cytotoxic effect; albeit, these toxic concentrations were not deemed to be biologically relevant. An effect of exposure time was observed for some experimental conditions. For example, cells were less viable and less metabolically active in a 72-hour exposure at lower monomer concentrations. Conclusion: This effort underscores the importance of bio-testing prior to comprehensive physicochemical/mechanical testing to ensure that the antimicrobial agent's potential cytotoxicity (to eukaryotic cells) is carefully balanced. We believe that this collective effort addresses a significant oral health issue associated with increased health risks in elderly populations. Its successful completion is expected to yield a new class of restoratives with well-controlled bio-function, a feature that has been marginalized in conventional class V restorative materials.
**Title of Talk:** Molecular Simulation of Semi-Crystalline Polymer Mechanics

**Abstract:**

Despite being one of the earliest studied types of polymers, semicrystalline polymers remain an ongoing theoretical and experimental challenge to characterize. The microstructure, or morphology, of these polymers consists of two types of regions—crystalline and amorphous. Although many techniques are available to characterize the crystalline domains (e.g., scattering, DSC, X-ray diffraction) these methods cannot easily be used to analyze the structure of the amorphous regions. Due to these limitations in metrology, our basic understanding of amorphous morphologies has mostly depended on theories rather than observation. However, as these theories have increasingly come into question, there has been a need to produce theoretical predictions that better relate to experimental measurements.

The goal of this research is to use large-scale coarse-grained simulations to understand how the microstructure of the crystalline and amorphous regions affects the mechanics of semicrystalline polymers. First, custom semicrystalline systems with designed crystalline and amorphous morphologies are generated using a Monte Carlo-based approach. Then, using Molecular Dynamics (MD) to simulate polymer deformations, we generate an ensemble of stress-strain data. Rather than relying on experimental techniques to directly characterize the amorphous topology of semicrystalline polymers, we can use simulated stress-strain data to predict semicrystalline morphology by comparison to experimentally generated stress-strain plots. Where the simulated and experimental data share qualitative similarities, we can infer that the structure of the real polymer might be similar to that of the simulated system. This study will enhance our understanding of the structure-property relationships for semicrystalline polymers, thereby helping materials scientists improve upon existing and future semicrystalline polymer systems.
Industrial polymeric network materials are often riddled with defects, and as a result are over-engineered and poorly understood at the molecular level. Here, we employ a bottlebrush polymer architecture, in network form, to access a family of crosslinked materials that are entirely entanglement free, allowing for the performance of fundamental mechanical and fracture studies which will better inform commercial synthesis and formulation.

Linear, low-dispersion acrylate ‘macromonomers’ were prepared via atom transfer radical polymerization (ATRP) and end functionalized by azidification of the bromine end groups, followed by a copper-catalyzed alkyne azide click reaction to affix a norbornene moiety. A second polymerization, ring opening metathesis polymerization (ROMP) linked these macromonomers through the olefinic norbornene groups to make a backbone of well-controlled length and dangling polymeric arms. Linear bottlebrush polymers were synthesized with degrees of polymerization (DP’s) up to 500 (Mn > 2,000,000 g/mol). These were imaged using Atomic Force Microscopy (AFM) in order to visually confirm the synthesis of such massive polymers. Crosslinked bottlebrush networks were also produced, where DP between crosslinks was varied by adding a precise ratio of di-functional macromonomer to the reaction. All materials were subject to adhesion testing and rheology in order to determine system information, most importantly modulus. Precision materials, such as these unentangled networks, are fundamental sources of information against which to compare non-ideal, swollen networks and gels made for commercial and industrial applications.
The increasing demand for plastic production along with improper waste management has created a significant accumulation of plastics in our world’s oceans. Several marine species have ingested these man-made polymers causing physical harm such as gut impaction or perforation. The possible impacts of toxic organic compounds leaching from these plastics into marine life is currently being investigated. Through identification and quantification of material properties of ocean plastics will aid these efforts and can contribute to understanding biological degradation mechanisms of polymers. The purpose of our study is to identify a series of plastics collected from beaches and the digestive tracts of sea turtles in Hawaii and measure their molar mass and other physical and chemical properties. Multiple methods were used in the identification and characterization process such as Gel Permeation Chromatography (GPC) and X-ray Photoelectron Spectroscopy (XPS). GPC separates the polymer molecules by their size providing number and weight average molar masses and molar mass distributions from refractive index (RI) and light scattering (LS) detection, as well as radius of gyration (from LS only). Additionally, infrared (IR) and viscometer signals gave short-chain branching and long-chain branching information, respectively. Sampling methods were optimized to ensure polymers were adequately dissolved and separated from biological contaminants for accurate analysis. Elemental composition data of the unknown polymers were measured by XPS to quantify carbon, oxygen, nitrogen, and chlorine content in the plastics. The samples are predominantly high density and low density polyethylene, whereas a small amount represents polystyrene and other theroplastics. Results of this investigation will help establish quantitative and systematic characterization practices for discarded plastics, yielding useful information for ecologists, materials scientists, industry, and governments to make insightful decisions regarding current ocean plastics, and support the design of future biodegradable materials.
**Abstract:**

Methanol is currently an important feedstock in the chemical industry, and recent work indicates that it may be used as a carbon source for olefin synthesis. It is also a potential fuel for use both in internal combustion engines and in direct methanol fuel cells. Methanol is currently produced through the reduction of CO/CO₂/H₂ (synthesis gas) over a Cu/ZnO/Al₂O₃ catalyst, but this process is low yielding (15% to 20%), requires harsh conditions, and catalyzes unwanted side reactions. Identifying alternative catalysts for methanol synthesis could facilitate environmentally friendly and economical production through CO₂ sequestration.

Though the exact mechanism of methanol synthesis is not known, the surface densities of the reactants, products, and intermediates on the catalyst play an important role in the overall rate of reaction. For this reason, the differences in binding energies of the various species could provide insight into the effectiveness of a catalyst. Calculating the binding energy is computationally simpler than constructing a full kinetic model, so in this project binding energy calculations will be used to examine a wide range of metals and metal alloys in order to identify promising potential catalysts that have not been considered in the past.

In my project, the binding energies of H₂, CO, CO₂, H₂O, and methanol on a zirconium surface were calculated. Powders of silver and zirconium were then synthesized and characterized using X-ray diffraction, thermogravimetric analysis, and volumetric gas uptake experiments. These experimental results were then compared to computational predictions.
Abstract:
The NBSR (National Bureau of Standards Reactor) is a heavy water moderated reactor, and as a result it produces tritium, a radioactive isotope of hydrogen that is dangerous when ingested. Inside the NCNR confinement building there exists a tritium monitoring system that samples the air of nine different pipes plumbed from different points in the building. The system samples air from each of these pipes, and sends the measured tritium levels to a display recorder in the reactor control room. Because of its ability to detect if there are any harmful leaks of radiation, the tritium monitoring system is crucial for safe operation of the NBSR. Like many industrial locales and nuclear reactor systems, the tritium monitoring system is controlled by a PLC (Programmable Logic Controller), which can communicate through a network, as well as automate many industrial processes. In addition to the PLC, a Digital Recorder actuates the valves that control the sample points, and displays trend graphs for the measured tritium levels and other components of the system.

The goal of my project was to take the existing tritium monitoring system and make changes such that the tasks done by the Digital Recorder, like valve actuation, are reassigned to the PLC for a more centralized, robust and versatile process control system. In addition, I used the Digital Recorder Software to customize the display and make my own configurations. In doing so I made the tritium monitor system more user friendly and readable, without losing any key functionality. To do this I had to learn in detail how the current system operates and how to configure and program industrial hardware. As a result, the NCNR has a more modern and capable tritium monitoring system, a small piece of the large effort to digitalize nuclear operations.

Title of Talk:
Tritium Air Monitoring System Refurbishment and Modernization

Pursuing a career in Computer Science or attending grad school somewhere.

NIST Laboratory, Division, and Group:
NIST Center for Neutron Research, Reactor Operations and Engineering Group.

NIST Research Advisor:
Dagistan Sahin

Future Plans (School/Career):
Pursuing a career in Computer Science or attending grad school somewhere.

Future Plans (Sept. '17):
To serve in Peace Corps for two years then return to graduate school for a Ph.D. in Computer Science. Then to work for a large technology company.

Title of Talk:
High throughput molecular dynamics for predicting the $\theta$-temperature of linear and ring polymers in solutions

Abstract:
Polymer scientists study the conformational properties of polymers in solution mainly as part of their characterization, but the solution properties are also very important in design of new materials, drag reducing agents, additives for water purification and in connection with stabilizing protein drugs and as thickeners in foods. Polymers, including their natural counterparts, proteins and DNA, exhibit three distinct classes of conformational ensembles, depending on the solubility of the chain segments in the solvent in which the polymer is dispersed. In a "good" solvent, flexible polymers swell due to the effective repulsive interactions between polymer segments, while in a "poor" solvent, the effective interactions between polymer segments become attractive, thus causing the chain to collapse. This leads to precipitation, which in most applications is an undesirable effect. At the boundary between "good" and "bad" solvent, the chain collapses into a droplet-like configuration. There is a marginal solvent regime near a $\theta$-solvent at which the repulsive and attractive interactions balance so the chain conformations are similar to an ideal random walk without losing any key functionality. To do this I had to learn in detail how the current system operates and how to configure and program industrial hardware. As a result, the NCNR has a more modern and capable tritium monitoring system, a small piece of the large effort to digitalize nuclear operations.

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**Title of Talk:** Fabrication of 2D material heterostructures by mechanical exfoliation towards phase-change devices

**Abstract:**

Transition metal dichalcogenides (TMDs) have become of great interest due to their potential applications in two-dimensional electronic devices. Molybdenum ditelluride (MoTe2) from the TMD family, exists in a metallic (1T') or semiconducting (2H) phase and exhibits a metal-to-semiconductor transition at elevated temperatures (above ~800°C). For practical device application, this transition temperature needs to be reduced, which we plan to explore by alloying MoTe2 with WTe2. However, a significant shortcoming of ultra-thin Mo(W)Te2 layers is their poor environmental stability, which causes material degradation upon air exposure. To combat this issue, Mo(W)Te2 thin layers need to be encapsulated with chemically inert material. Hexagonal Boron nitride (hBN), which is also electrically insulating, is perfect for this purpose.

In this project, a novel technique for the encapsulation of MoTe2 and Mo(W)Te2 alloys with hBN was developed by exfoliation of thin layers with follow-up mechanical stacking. The fabrication of hBN/Mo(W)Te2/hBN heterostructures on Si/SiO2 substrate was characterized with optical, Raman, scanning electron and atomic force microscopies. Then, the effects of alloying MoTe2 with tungsten on the metal-to-semiconductor transition temperature were investigated by annealing encapsulated BN/Mo(W)Te2/BN stacks in the temperature range of 400°C to 950°C in argon. Thermal stability of Mo(W)Te2 alloys, including compositional dependence of the 1T'-2H phase change temperature, was monitored by SEM/EDS and Raman spectroscopy.

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**Title of Talk:** Advanced Design of Octo-Strain Device for Multi-Axial Sheet Metal Testing using in-situ Neutron Diffraction

**Abstract:**

Recent advancements in the mechanical properties of sheet metal have led to the development of refined mechanical testing methods. Automotive lightweighting research is critical to meet consumer demand to develop automobiles with increased fuel efficiency, while improving crash test ratings. The goal of this research was to design an Octo-Strain device that will be used to standardize measurement techniques using in-situ neutron diffraction to measure the stress of the material. This data, along with strain data is used create material models that accurately represent the microstructure of the material.

To develop an Octo-Strain device, 3D Computer-Aided Design software (CAD) was used to create an assembly drawing of all components. Finite Element Analysis software (FEA) was used to ensure the device would meet stiffness requirements with maximum tensile and compression loading conditions. In addition, this design uses a pulley and timing belt configuration to drive the eight linear actuators. Torque calculations were performed to ensure the belt and pulley could apply the required 50 kN force without slippage to each of the eight loading arms.

The result is a completed professional design of an Octo-Strain device that triples the load capacity of the current system and allows for multi-axial loading. By using the pulley and belt drive system, significant space is saved. This allows for an increased range of measurable scattering angles. When this design is assembled, experiments will be conducted to provide accurate data of the material properties. With these data, the automotive industry will be able to save costs and benefit the consumer through successful product development.
Title of Talk: Latent Fingerprint Developer Standards Development

Abstract:

For decades ninhydrin has dominated forensic laboratories as the chemical of choice for latent fingerprint development on porous substrates due to its inexpensiveness, universality, and practical developing technique. This simple developing process is based on the reaction of ninhydrin with the multiple amino acids present in fingerprint deposits to produce a compound with a distinctive purple color. Because of its widespread usage, it is of utmost importance for forensic laboratories to be confident that the ninhydrin being used is able to develop fingerprints as required. This research continues the efforts of constructing a standard method to determine the stability and efficacy of ninhydrin and of other types of fingerprint developing agents. Liquid chromatography mass spectrometry (LC/MS) was utilized to quantify the stability of ninhydrin under different storage conditions as well as to analyze its degradation products. Results from this analysis have been compared to previous studies that have used different analytical techniques such as gas chromatography mass spectrometry (GC/MS) and ultraviolet-visible spectroscopy (UV-Vis). Furthermore, investigation of the stability of ninhydrin under different conditions allowed for the determination of the optimal storage option for the developing agent. The efficacy of ninhydrin was also evaluated over time by producing inkjet-printed amino acid test strips and monitoring the extent of the developing agent’s reaction with the deposited amino acids. The piezoelectric inkjet printer ensured the deposition of a precise amount of material onto the substrate, and, through measuring the color of the developed test strips, the efficacy of ninhydrin was quantified. This work will help provide the forensic community with a quality control mechanism for ninhydrin as well as for other reagents thus allowing laboratories to have confidence in their latent fingerprint developing process.

Title of Talk: Substrate Influence on Hygro-mechanical response of Nafion Membranes

Abstract:

Proton Exchange Membrane (PEM) fuel cells are candidates to serve as an alternative fuel source in the transportation industry, and Nafion is the state-of-the-art polymer used and researched for this application. Understanding the mechanical properties of Nafion is critical because the membrane must be mechanically robust to prevent reactant gas crossover and withstand the swelling stresses associated with hydration during operation. Water is used to facilitate proton conductivity in Nafion, therefore it is important to understand how the mechanical properties and swelling stresses vary with water content. In addition to the PEM, Nafion is also used as an ion-conducting binder in the catalyst layer. Within the catalyst layer, Nafion forms a coating on carbon and platinum nanoparticles on the order of 10 nm. In this project, a cantilever bending technique developed at NIST was used to determine mechanical properties of Nafion films of thicknesses from 300 nm to 45 nm on a variety of substrates.

There was no significant influence of the substrate material on the mechanical properties of Nafion films greater than 200 nm thick. Upon annealing at temperatures above 100 °C the Young’s Modulus increased by a factor of five due to an increase in the crystallinity and physical crosslinking. In thin films, substrate material had a significant impact on the resultant mechanical properties. A 50 nm thick Nafion film on platinum had a Young’s modulus four times greater than that on gold and silicon. The measured stress values approaching 50 MPa, three times larger than the reported yield stress of bulk Nafion, call into question the durability of a thin Nafion film on platinum. The cantilever experiments indicated no sign of plastic deformation or yielding, but further testing of the cyclability of these membranes is necessary to determine if thin membranes can withstand repeated stress cycles.
Stainless steels are alloys that can potentially consist of many different phases within the material: ferrite, which contributes to high elongation but low strength, martensite which provides high strength but low ductility, and austenite, which can exhibit high elongation and strength depending on the operative deformation mechanisms. Austenite can undergo a strain-induced transformation to martensite (transformation induced plasticity or TRIP effect) during plastic deformation, which can lead to increased work hardening and delayed necking. Understanding and controlling this transformation is valuable for developing and implementing advanced high strength steels (AHSS) in industry; therefore, it is vital to accurately evaluate the austenite content in steel.

X-ray diffraction (XRD) is a widely utilized method for conducting phase fraction analysis. However, during XRD of steel samples, the crystallographic texture is often ignored. This can create large errors in the exact volume percent of austenite present. The presence of texture due to processing of the steel and the change in texture during deformation make it difficult to gather information about how strain affects the austenite content in a sample due to the TRIP mechanism.

One approach to this problem is to perform XRD on a different geometric surface rather than in one of the more common directions (i.e. normal, transverse and rolling directions). A cube shaped sample cut along the (111) plane combined with collecting data over many different sample orientations could eliminate the texture bias error during XRD analysis, leading to more accurate phase fractions.

By dealing with texture in this way, it is then possible to obtain accurate data on how phase fractions relate to plastic deformation behavior in stainless steels. Tension and compression tests were conducted to place various amounts of retained strain within the steel. Then by using XRD, austenite content was measured as a function of strain, leading to a greater understanding as to how AHSS respond to deformation.
Title of Talk: Analysis of Polymer Thin Films for Organic Photovoltaics Through In-situ Spectroscopic Ellipsometry, or How I Learned to Watch Paint Dry

Abstract:

Organic field effect transistors and photovoltaics have gained significant interest over the past few years due to the numerous applications and potential to replace certain silicon systems. Furthermore, this set of materials are relatively cheap and easy to produce from an industrial standpoint as these materials can be processed using roll-to-roll techniques such as slot-die coating and inkjet printing. Recent research efforts have focused on the characterization of organic semiconducting molecules and polymers and polymer blends that exhibit varying levels of self-alignment and form multiple layers when coated onto a substrate. Two small molecule:polymer blends that potentially exhibit segregation of one of the components at either the air or substrate interface, BTBT:IDTBT and difTES-ADT:PTAA, were the primary focus of this study.

Thin films were fabricated using a solution deposition technique known as blade coating. This technique has been previously shown to be equivalent to industrial scale slot-die coating. Film formation was studied during the coating process using grazing incidence wide angle X-ray scattering (GIWAXS) and spectroscopic ellipsometry (SE). These two methods provide data that can then be analyzed to identify notable features that develop as the solvent dries. Specifically, the data can be used to identify when during film formation different phases occur. This in part can create desired physical properties, such as high stability and monodispersity of the silver nanoparticles.
Title of Talk: Measurement of Interfacial Tension of Polyelectrolyte Complex Coacervates

Abstract:

Polyelectrolytes are polymers whose repeating subunits contain an electrolyte group. Complex coacervation occurs when a solution of two oppositely charged polyelectrolytes undergoes liquid-liquid phase separation under suitable conditions. The coacervate, the polymer-rich phase coexisting with the polymer-poor supernatant, is known to exhibit viscoelasticity and very low interfacial tension. Due to these interesting properties, coacervates have great potential for various biomedical applications such as in drug delivery, scaffold formation and wet adhesives. Such applications require accurate measurement of the low interfacial tension of these systems at various physicochemical conditions. This project used drop-retraction analysis which has been developed to estimate the low interfacial tension of coacervates at varying salt concentrations, molecular weights and temperatures. In this method, micron-sized droplets of dilute aqueous-phase are generated in the coacervate domain. These droplets are then deformed by applying controlled shear rates using a shear cell. Subsequently, the retraction of these droplets as a function of time at zero-shear condition are captured using a microscope and the deformation parameters are then calculated using an automated image analysis method. This data is further analyzed using existing theory to calculate the interfacial tension. We believe that this method offers several advantages over other existing techniques to estimate ultra-low interfacial tension of coacervates at varying physicochemical conditions relevant to various practical applications.
Cabrera, Lauren - PML-PL
Calamari, Justin - PML-PL
Capric, Suzanna - PML-EE
Chavali, Sai-Meghasena - PML-EE
Davis, Robert - PML-EE
DiBernardo, Emma - PML-EE
Edgerton, Joshua - PML-PL
Ford, Joni - PML-EE
Hanson, Edward - PML-EE
Hanson, Joshua - PML-PL
Kasik, Camden - PML-PL
Miller, Hallie - PML-PL
Montgomery, Karl - PML-EE
Moore, Rebecca - PML-EE
Motabar, Lily - PML-EE
Mullins, David - PML-PL
Murthy, Vaishnavi - PML-EE
Nacion, Edsel - PML-EE
Neice, Claire - PML-PL
Oler, Daniel - PML-EE
Perez, Alondra - PML-EE
Phan, Nhi - PML-EE
Regan, Malcolm - PML-EE
Shlosberg, Ariel - PML-PL
Streater, Richelle - PML-PL
Terranova, Nicholas - PML-PL
Vang, Doua - PML-EE
Waldron, Zachary - PML-PL
Zaytoun, Christian - PML-PL
Zhou, Peter - PML-PL
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Luke Amatucci
Academic Institution: Boston University
Grant Number: 70NANB16H164

Title of Talk: Characterization of Miniature Differential Pressure Sensors

Abstract:
NIST Fluid Metrology Group is currently running a project connected with flow measurement in large smokestacks. Accurate measurements of flows in smokestacks of coal-burning power plants are needed to better control pollutants emitted by these plants. The Electric Power Research Institute hopes to achieve measurement uncertainties near 1%. To achieve accurate flow measurements with expanded uncertainty of 1%-2%, industry uses 2D and 3D multi-hole Pitot tubes. Using these probes requires up to 6 differential pressure measurements to be taken at once. The differential pressure readings can then be converted to velocity as well as pitch and yaw angles of the flow. The system consists of the 3D Pitot tube probe, data acquisition system, and data processing to compute velocity, yaw, and pitch angles. For this system, miniature differential pressure sensors are ideal for collecting pressure data from multiple ports. The Scanivalve 2033 sensor and miniature differential pressure sensors from Honeywell were tested. LabVIEW software to collect data was developed and integrated into existing airspeed primary calibration facility systems. The miniature differential pressure sensors were then tested for sensitivity, stability, and zero-drift. The performance of the sensors was tested using the NIST Wind Tunnel to measure differential pressure of a spherical 3D probe at different pitch, yaw, and airspeed values. It was found that the difference between airspeed measured by NIST differential pressure standards and mini-sensors was less than 0.4%; difference in pitch, less than 0.5°. Based on wind tunnel test results a suitable miniature pressure sensor will be chosen to be used in conjunction with 3D Pitot tubes in the future for improved quality of flow measurements in the field.

Future Plans:
Pursuing a career in fluid dynamics research.

Advisor:
Lauren Cabrera

Title of Talk: Into the Woods: A look into urban forest carbon dynamics

Abstract:
Our understanding of the role forests play in the global terrestrial carbon cycle has largely been based on rural intact forests. Studying urban forests is becoming increasingly important as growing portion of the planet’s forests becomes more fragmented with the anticipated global environmental changes. New research suggests that remotely sensed solar-induced fluorescence (SIF) can be efficient way to measure forest productivity, both on a broad spatial scale and at a high frequency. The National Institute of Science and Technology (NIST) campus provides the perfect place to measure small scale forest data and larger scale remotely sensed data, as well as their relationships, because it is a suburban fragmented forest surrounded with some of the best measurement technology in the world.

The research is taking place in a 100m x 100m plot of temperate hardwood forest on the west side of NIST’s campus. Variables such as tree growth, tree sap flux, tree and soil carbon flux, canopy leaf area, and micrometeorological data are measured on a small-scale basis. Through statistical and regression analysis, they are then correlated to large scale measurements taken by sensors such as hyperspectral imagers, thermal infrared sensors, SIF sensors, LiDAR imagers, and pulse amplitude modulated (PAM) chlorophyll fluorimeters. Thus far, tree growth, tree respiration, and soil respiration measurements have been collected on a weekly basis. Tree sap flux, soil moisture, and air temperature and humidity measurements are being logged on a minute by minute scale. A camera takes phenological observations every 15 minutes and a 3D model of the forest edge has been constructed by LiDAR. Further hyperspectral, thermal, and SIF measurements are planned. In preliminary data, stem respiration has shown correlations to both tree size and growth rate. While there are strong spatial variations from the edge of the forest in relation to air temperature, there are low spatial variations in soil respiration. Soil respiration is also at much higher rates than stem respiration. In the future, these will be linked to remotely sensed data and can hopefully be used to describe forests on large spatial scales.
**Title of Talk:** Construction of 2D and 3D Magneto-Optical Traps for Lithium and Rubidium Atoms

**Abstract:**
NIST is developing a new standard for ultra-high (UHV) and extreme-high vacuum (XHV) measurements. The standard is based on the loss rates of cold atoms in a magnetic trap due to collisions with background gas in the vacuum. To achieve this, multiple steps of laser cooling with different types of traps and geometries are required in order to reach the necessary sub-millikelvin temperatures. The workhorse in this field is the magneto-optical trap (MOT), which uses laser cooling combined with a magnetic field gradient to provide spatial confinement. Once cooled in a MOT, atoms are transferred into a purely magnetic trap, and remain in place until a background gas collision.

In our experiment, Li or Rb atoms are vaporized and loaded into a MOT along two spatial directions (a 2D MOT), which redirects the atoms into a collimated beam. The beam passes into a sensing chamber where atoms are captured by a MOT in three spatial directions (a 3D MOT). Once cooled, the lasers are turned off and the magnetic field configuration is changed from a quadrupole field needed for the MOT to a Ioffe-Pritchard magnetic trap, and the atoms begin sensing background gas.

In this research, we construct 2D and 3D MOTs for lithium and rubidium atoms. We align laser beams, lock the laser frequencies, and set up optics necessary to collimate and polarize the laser-cooling beams. We use both permanent magnets and electromagnets for the MOTs so currents can be adjusted to change between a Li and Rb MOT. This summer, we achieved a 2D MOT for Li and are preparing to test the Li 3D MOT. We also test a chip-scale version of this apparatus containing MOT coils compressed into a plane. This research will help realize a primary standard and develop absolute sensors for UHV and XHV.
**Name:** Sai Meghavendra Chavali  
**Grant Number:** 70NANB16H  
**Academic Institution:** University of Maryland  
**Major:** Electrical Engineering  
**Future Plans (School/Career):** Graduate School  
**Synopsis:** Analysis of Neutron Beam Images for a Neutron Lifetime Experiment  

**Abstract:**

Measuring the neutron lifetime is an important way to test the Standard Model of particle physics and provide insight about the early evolution of elements in the cosmos. To improve the precision of the neutron lifetime value and understand systematic uncertainties, we are conducting a new experiment using the beam method at the NIST Center for Neutron Research (NCNR). In order to measure the neutron lifetime using the beam method, it is necessary to know the number of neutrons, the size of the proton trap volume, and the number of protons resulting from neutron decay. To accurately count the number of protons, one must first determine the neutron beam size and distribution by taking images of the neutron beam. In my presentation, I will present these images, discuss the image analysis necessary to determine the size of the neutron beam, and explain how this analysis helps us with the neutron lifetime experiment.

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**Name:** Robert Davis  
**Grant Number:** 70NANB16H  
**Academic Institution:** University of Colorado Boulder  
**Major:** Electrical Engineering  
**Future Plans (School/Career):** Graduate school for a Ph.D. in electrical engineering, and eventually a career in research  
**Synopsis:** Laser Frequency Stability and Photonic Crystal Membrane Characterization  

**Abstract:**

In precision interferometry, an important technique involves relating small displacements to a corresponding wavelength of a probe laser. Because the optical frequency of the laser is directly related to the measurement result, an understanding of the laser’s frequency stability is of great interest. Similarly, these types of measurements rely on photodetectors, which are affected by intensity noise of the laser. Relating this intensity noise to the quantum shot noise limit helps one understand the relative quality of measurements. For the first stage of this project, I performed a rigorous analysis of the frequency stability and intensity noise of three commercial telecommunications lasers. Using the Allan deviation as a measure of frequency stability, the results indicate that all three lasers exhibit white noise limited behavior under short (millisecond) time intervals.

Making use of this knowledge, the second stage of the project focused on the characterization of a silicon nitride photonic crystal membrane. The membrane itself is an ultrathin array of holes intended for optomechanics purposes, which acts like a diffraction grating. We first explored a novel approach for measuring the grating period by placing the membrane in a Littrow configuration and recording the reflection angle on a Vernier scale. By exploiting the accuracy of a laser wavelength reference and measuring up to the fourth diffraction order, the period was calculated to be very close to measurements taken with a SEM, but with a better relative uncertainty. The next step will be to place the membrane inside a vacuum chamber and use it as one leg of a Michelson interferometer to record its thermal movement. This will provide useful mechanical resonance information for future optomechanical experiments.
In recent years, the digital smart watt-hour meter has replaced the traditional electromechanical watt-hour meter in residences, businesses and industries for more reliable and accurate electricity metering. While the smart meter has proven more dependable than the traditional electricity meter, the smart meter may still be vulnerable to inaccuracies when measuring non-linear loads, power loads that produce high ordered harmonics causing a distorted power signal. These inaccuracies can cause discrepancies in electricity bills for consumers.

We have designed a test setup to determine how distortions from common non-linear loads affect smart meter reading accuracies. In this design, up to eight smart meters will read the power generated from a combination of normal and distorted power signals accurately to improve the digital smart meter standard and provide a more dependable instrument for consumers.

The most dramatic improvements occurred for sources that had activities between 2.5 kBq and 11 kBq, especially when paired with booster sources that had activities of 15 kBq to 27 kBq. For the VIC, bias was greatly reduced for the weaker sources from 20% to less than 5%. For the CRC-15R, the booster method reduced the bias in the weak source measurements from 15% to less than 5% for the lowest activity sources. The most dramatic improvements occurred for sources that had activities between 2.5 kBq and 11 kBq, especially when paired with booster sources that had activities of 15 kBq to 27 kBq. For the VIC, bias was greatly reduced for the weaker sources from 20% to less than 5%. The stronger sources also had a reduction in bias, with a comparable uncertainty to the measurement of the single source. In general, the uncertainties present in the activities produced by the booster method were large but could be reduced by taking a larger number of measurements, especially in the CRC-15R. Accurate measurement of lower activity sources using the booster method could provide a cheap and quick way of extending the range of clinically used ionization chambers, which means that life-saving advances in nuclear medicine can reach patients faster.

We have designed a test setup to determine how distortions from common non-linear loads affect smart meter reading accuracies. In this design, up to eight smart meters will read the power generated from a combination of normal and distorted power signals accurately to improve the digital smart meter standard and provide a more dependable instrument for consumers.

Title of Talk: The Booster Method: Extending the Range of Ionization Chambers for Pre-Clinical Trials

Abstract:

Reentrant ionization chambers are vital instruments in nuclear medicine. They measure the activity of radiopharmaceuticals used for treatment and imaging. Accurate measurement of the activity is dependent on the assumption that there is a linear response for all activities. However, for very small or very large activities, the response becomes nonlinear. Since small activities are used in pre-clinical trials for positron emission tomography (PET) and single photon emission computed tomography (SPECT) involving animals, a method to reduce the bias on small measurements is desirable. One proposed solution is to introduce an additional "booster" source in the ionization chamber so that the combined activity falls in the range of linear response. The booster activity could then be subtracted from the total read activity to recover the activity of the weaker source. The booster method was performed using Ge-68 sources of varying activities in two dose calibrators, the Capintec Radiosotope Calibrator (CRC-15R) and the Vinten Ionization Chamber (VIC), to provide a proof-of-concept. For the CRC-15R, the booster method reduced the bias in the weak source measurements from 15% to less than 5% for the lowest activity sources. The most dramatic improvements occurred for sources that had activities between 2.5 kBq and 11 kBq, especially when paired with booster sources that had activities of 15 kBq to 27 kBq. For the VIC, bias was greatly reduced for the weaker sources from 20% to less than 5%. The stronger sources also had a reduction in bias, with a comparable uncertainty to the measurement of the single source. In general, the uncertainties present in the activities produced by the booster method were large but could be reduced by taking a larger number of measurements, especially in the CRC-15R. Accurate measurement of lower activity sources using the booster method could provide a cheap and quick way of extending the range of clinically used ionization chambers, which means that life-saving advances in nuclear medicine can reach patients faster.
**Abstract:**

Optical fibers are flexible waveguides that can transmit light with very little loss of strength. When a Fiber Bragg Grating (FBG) is constructed onto an optical fiber, specific wavelengths are reflected and can be monitored. Whenever a FBG experiences strain or a change of temperature, the reflected wavelength will shift to reflect this change. Thus, FBG sensors can be used in a plethora of metrology applications, since they can be embedded into virtually any material that can contain a fiber, and can be used to make a wide variety of measurements from humidity to dynamic pressure.

The purpose of my project is to utilize FBGs' flexibility to take a wide variety of real-time measurements. For one application, a FBG is embedded into Polydimethylsiloxane (PDMS)—a polymer with squishy characteristics—to mimic a human vein. Another application involves using FBGs embedded into concrete to track expansion and changes in humidity and temperature as the concrete cures as well as when the concrete experiences immense stress while being crushed. Through these experiments, I aim to demonstrate the accuracy and dependability of photonic sensors within a variety of applications.
Abstract:
Moving from a physical standard realized at NIST to a deployable product that realizes that standard generally involves scaling down a laboratory experiment into a much smaller package. This concept holds true for standards and gauges based on laser-cooled alkali atoms. To achieve laser cooling, there must first be an appreciable number of room temperature atoms inside a vacuum system from which a small fraction will be cooled. Traditionally this is done by heating an alkali metal source to high temperature, about 100°C for rubidium and 400°C for lithium. This generally requires bulky objects like heaters and can cause outgassing which spoils the properties of the vacuum. Light induced atomic desorption (LIAD), on the other hand, has the capability to eject sufficient numbers of rubidium and lithium atoms into the vacuum while circumventing the heating process. The theory behind LIAD is not fully understood, but it is known from experiments that LIAD occurs by shining light onto a surface where atoms have been absorbed, causing the originally absorbed atoms to travel away from the surface. In this project, the rate of atomic desorption was measured by directing light from a light emitting diode (LED) towards a glass window coated with rubidium or lithium atoms. The desorbed atoms accelerated into a residual gas analyzer (RGA), where we determined the increase in the partial pressure of the alkali gas. The power of the LED’s light was measured simultaneously to correct for any long-time drifts in the LED power. We measured the relationship between the intensity, wavelength, and angle of the incident light to the rate of desorption among different alkali metals. In the future LIAD could be used in miniature laser cooling or vacuum standard products to make the atom source reusable and eliminate the need for heating.
The continual progress of research requires that the corresponding metrological tools become more sophisticated and specialized to keep up with the ever-increasing demands placed on them. It is imperative that researchers understand not only how to use a specific piece of hardware or software, but also the principles governing how it works so more intricate systems may be conceived, created, and manipulated to pursue groundbreaking experimentation. Such skills are foundational at metrology institutes such as the National Institute of Standards and Technology (NIST) where cutting-edge facilities are the norm.

In 2016, NIST’s Nanoelectronics Group designed and constructed a one-of-a-kind magneto-Raman system with the capability to perform in operando spectroscopy. Measurements can take place at cryogenic temperatures with control of both magnetic and electric fields, using tunable laser wavelengths and piezoelectric positioning of samples. The apparatus can now use Raman spectroscopy to map or image the sample while it is under a complex parameter space, investigating variables such as temperature, electric field, magnetic field, and excitation wavelength. The new automation will save time and allow NIST scientists to pursue in operando spectroscopic research imperative to the development of the next generation of nanoscale electronics.

Certain commercial equipment, instruments, or materials are identified in this paper in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

In our project, we have created biomaterial scaffolds via layer-by-layer deposition of polyelectrolytes onto positively charged microparticles (beads) packed within microfluidic channels in polymethylsiloxane (PDMS) devices. Microfluidic systems offer higher compaction and less displacement of beads, leading to better formed scaffolds. We used polyelectrolytes found in the body: hyaluronic acid (HA), a major component of the ECM in all tissue, and poly-L-Lysine (PLL), a polypeptide polycation. The number of layers, as well as the final layer, on the substrate were varied to observe the effect on cell morphology of HepG2 human liver cancer cells. When grown on a polystyrene dish with no cell adhesive layer or a single layer of anionic HA, the cells appear more aggregated; when grown on a single layer of cationic PLL or multiple layers of alternating HA and PLL, the cells are more dispersed. Our project demonstrates that layer-by-layer deposition of materials provides a method to construct biomimetic ECM substitutes with nanoscale control of layer thickness and architecture. In addition, using ECM components as an in vitro substrate influences cell behavior and gives additional insight into how cells would behave in a more physiologically relevant microenvironment.
Name: David Andrew Mullins  
Academic Institution: University of Kentucky  
Major: Physics  
Grant Number: 70NANB16H123  
Academic Standing (Sept. '17): Senior  
Future Plans (School/Career): I would like to attend graduate school for physics  
NIST Laboratory, Division, and Group: NIST Center for Neutron Research, Physical Measurement Laboratory, Neutron Physics  
NIST Research Advisor: Daniel Hussey  
Title of Talk: Neutron Dark-Field Imaging  

Abstract: 
Neutron imaging is typically used to image and reconstruct objects that are difficult to image using X-Ray imaging techniques. X-Ray absorption is primarily determined by the electron density of the material. This makes it difficult to image objects within materials that have high densities such as metal. However, the neutron scattering cross-section primarily depends on the strong nuclear force, which varies somewhat randomly across the periodic table. In this project, an imaging technique known as far-field interferometry has been used to study a sample of granite. With this technique, interferometric phase images are generated. The dispersion of the microstructure of the sample dephases the beam, reducing the visibility. Collecting tomographic projections at different autocorrelation lengths (from 100 nm to 1.74 μm) essentially creates a 3D small angle scattering pattern, enabling mapping of how the microstructure is distributed throughout the sample.

Name: Vaishnavi Murthy  
Academic Institution: University of Maryland, College Park  
Major: Electrical Engineering  
Grant Number: 70NANB16H  
Academic Standing (Sept. '17): Junior  
Future Plans (School/Career): Graduate Studies  
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Quantum Measurement Division, Mass and Force Group  
NIST Research Advisor: Patrick Abbott, Edward Mulhern, Corey Stambaugh  
Title of Talk: Development of an Arduino-based Humidity Control System for regulating the environment of a mass artifact storage chamber  

Abstract: 
Beginning in 2019, NIST will disseminate the unit of mass from two ensembles of mass artifacts: one ensemble will be maintained in atmospheric pressure air and the other will be maintained under vacuum at a pressure of approximately 10^-3 Pa. For the ensemble stored in air, it is critical that the pressure, temperature, and relative humidity are controlled within certain limits to ensure stability of the mass artifacts.

Because humidity is the most variable parameter of these three, in this project, we have developed a microcontroller-based humidity control system that uses the “bubbler method” to maintain the relative humidity inside the chamber. With this technique, we can send dry or humidified air to the chamber via two solenoid valves that are managed by the microcontroller. By using a proportional-integral-derivative (PID) control loop, the microcontroller regulates the flow of dry and humidified air through the two valves to maintain the relative humidity inside the chamber to within +/-1 % of the set value. The PID algorithm uses adjustable tuning parameters and sampling frequency to achieve the most accurate and precise results as possible. Additionally, to ensure that the pressure inside the test chamber does not become too high, we have added a third outflow solenoid valve that opens whenever humid or dry air enters the chamber. Otherwise, the outflow valve is closed to prevent the entry of contaminants from the outside world.

By choosing to build our own controller instead of using an expensive commercial product that would have the same function, we are able to confirm the ability of low-cost microcontrollers to perform high-level metrology with a low uncertainty.
**Title of Talk:** Transport Measurement of 2-Dimensional Nanoelectronic Devices

**Abstract:**

2-dimensional transition-metal dichalcogenides (2D-TMD) such as MoS$_2$ and WSe$_2$ have been studied as promising candidates for future high-performance computing and flexible electronic devices. Precisely controlling the doping level of these materials is still a challenge. This project aims to use an ionic liquid gating technique to electrostatically control doping levels of 2D-TMDs and improve the device characteristics for high-performance switching applications.

Tunable laser diodes offer wide applicability. However, certain applications require accurate and precise laser frequencies. Thus, feedback systems have been developed. Typical feedback systems compare a laser’s frequency to that of a reference, then feed the error between them to a laser controller. This drives the laser towards the desired reference frequency. These laser stabilization systems, also called locks, are often based on proportional-integral-derivative (PID) servo controllers. Several types of locks exist, including a side lock, dither lock, Pound-Drever-Hall (PDH) lock, and Hänsch-Couillaud lock. These rely on several large, scientific grade instruments, such as a servo controller, lock-in amplifier, function generator, and oscilloscope. We are developing a National Instruments Labview programmed field programmable gate array (FPGA) based laser stabilization technique to eliminate the need for some or all of these instruments.

To test the performance of our device, we compared the traditional dither lock, FPGA-based dither lock, PDH lock, and FPGA-based PDH lock methods for locking a telcom distributed feedback laser (DFB) to P(1) of the hydrogen cyanide (H$^1$C$^3$N)$_2$ rotational-vibrational combination band near 1542 nm. This resulted in frequency lock errors of 4.2 MHz, 5.1 MHz, and 1.7 MHz, respectively measured over five minutes. The FPGA-based PDH lock is currently being characterized and the results will be presented. We will begin integrating this system into various projects in our lab, as well as transporting it to other labs to make measurements using photonic sensors. This laser stabilization system offers a robust, deployable, and cost-effective alternative to traditional, analog systems, a major advancement for the NIST-on-a-Chip program.
Title of Talk: Automation of the Ultra-Low Current Amplifier (ULCA) System for the Calibration of femto-amp meters

Abstract:
An interest for accurate measurements of sub-nanoparticle currents have increased in fundamental metrology, requiring calibration of picoampere meters and low-current sources. The Metrology of the Ohm project is responsible for accurate calibration of resistance standards ranging from micro-ohms to tera-ohms. Accurate calibration of high resistance standards relies on transfer standards, resistance bridges, and precise low current measurements using femto-amp meters. Furthermore, the Metrology of the Ohm project’s ongoing support for electrical traceability requires generation of low currents with substantially low uncertainties. These projects include support for the US Army for the aerosol electrometers (±20 fA to ±40 fA), the NIST Optical Technology Division for photodetectors (±10 pA to ±10 uA), and the NIST Ionization Radiation Division for dosimeters (±1 pA to ±200 nA). To characterize femto-amp meters and to generate low currents with substantially low uncertainties than currently achievable, an Ultra-Low Current Amplifier (ULCA) system is introduced. The ULCA is a transresistance amplifier for measuring small electric currents. In combination with an additional voltage source (waveform generator), the ULCA can also be used to generate small currents. The focus of this project has been to develop a LabVIEW program to automate the ULCA system to generate and source currents. The program was used to calibrate femto-amp source meters using measurement and generation modes of the system. Calibrations were performed in both ±1 fA ±1 ±5 nA and ±5 nA ±1 ±5 μA ranges. The results from the data collected will help improve measurement techniques for several low current applications traceable to electrical quantum standards.

Title of Talk: Assembly of a Dedicated Quantitative Imager for Fluorescence and Bioluminescence

Abstract:
Fluorescence and bioluminescence markers have been rapidly adapted for fluorescence-guided surgery (FGS) and other interventions. Innovations in surgical visualization include improvement in pathological lesion detection for ablation procedures and thereby potentially eliminating the need for lymph node biopsies for diagnosis of breast and prostate cancers. The emerging utility of FGS in the biomedical field calls for the development of standards that would allow for the evaluation of fluorescence imaging responsivity across different imaging systems to ensure the effectiveness and safety of such systems. Currently, there is no universal standard for fluorescence imaging systems, leading to performance results which are not readily comparable between different imaging systems. Preclinical researchers and fluorescence imaging developers routinely utilize polymeric materials with embedded fluorophores and scatterers to mimic fluorescence in tissues. These so-called tissue phantoms are presented to an imager and serves as a daily calibrator of imaging systems. We utilize the invariance property of radiance as a method to transfer calibration between different imaging systems. To validate this proposed technique as an alternative to irradiance-based calibration, we evaluated the response of two separate detector systems to a 850nm fiber-coupled light source with the purpose of creating an optical scale that relates intensity counts given by the detector to the radiance of the light source as measured by a NIST-calibrated photodiode. This non-clinical method of imager performance evaluation would provide researchers and medical professionals with SI-traceable optical measurements that will ultimately lead to quantitative measurement of the fluorescent substance, which is proportional to the disease biomarker being investigated.
Abstract:

Instruments and methods which measure the nanometer scale electrical properties of materials have made possible the rapid design and manufacture of countless valuable technologies. Improving the precision of these measurement techniques could stimulate further development of future computing devices and provide new insights into current engineering problems. However, because the measuring probe becomes a component of the system it measures, the measurement's precision is limited by how well the electrical shape of the probe is known. Knowledge of this electrical shape – which refers to the spatial distribution of electrical quantities about the probe due to its geometry, materials of construction, and position in the system – could be used to refine instrument calibration procedures or to inform the design of a probe which minimally disturbs the system it measures. In general, information pertaining to the electrical shape is elusive in that it must be found via numerical methods.

Experimentally, it has been observed that Scanning Kelvin Force Microscopy (SKFM) measurements of structures with abrupt boundaries in potential are dependent on the tip shape and the angle of approach of the tip, implying that the tip shape is convoluted with the SKFM response. This project investigates methods to extract the electrical shape of a probe from surface potential measurements of a sample with known potential profile. The SKFM measurement has been simulated in two- and three-dimensions using the COMSOL MultiPhysics software with a realistic model of the tip, cantilever, and experimental test structures. It was found that a basic estimate of the two-dimensional tip shape can be obtained from the measured contact potential difference (CPD) versus position curves using an analytical expression derived from comparing simulated SKFM profiles with the tip shape used in the simulation. Experimentally, SKFM was used to measure the CPD between the probe and the sample as the probe is scanned over a gold-platinum interface at 90, 45, 0, and -45 degrees using various shapes of commercially available probe tips, including a co-axially shielded probe tip. To improve the initial estimate of the probe tip shape, the initial estimate is parameterized and used in a 2nd COMSOL simulation of the response. The difference between the simulated and measured CPD response are then used to adjust the probe shape estimate.

* Certain commercial equipment, instruments, or materials are identified in this paper in order to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by NIST, nor does it imply that the materials or equipment are necessarily the best available for the purpose.
**Title of Talk:** Diffuse Optical Properties of a Solid Reference Standard for Biomedical Optics

**Abstract:**

In biomedical optics, solid reference objects or “phantoms” are useful in simulating light propagation through human tissue. To create an accurate simulation, a phantom and the tissue it is mimicking must have similar absorption and scattering coefficients ($\mu_a$ and $\mu_s$). NIST aims to standardize the measurement of these coefficients, which in part involves the development of a program to solve for $\mu_a$ and $\mu_s$ given experimental angle-resolved scattering (ARS) data. Previous NIST research has accomplished this through a log-likelihood search algorithm with Monte Carlo forward simulations, with a time-to-solution of about two hours. This summer’s research successfully implemented importance sampling on top of this approach.

The current program inputs an experimental ARS curve and a starting set of possible $\mu_a$ and $\mu_s$ values. It runs a forward Monte Carlo ARS simulation with the middle point of the $\mu_a$ - $\mu_s$ grid as its reference parameters. The importance sampling algorithm weights the reference ARS curve to determine the curve for each point in the parameter space. The program then calculates the log-likelihood for each fit and shrinks the search area down to the points within a threshold confidence. It then repeats all steps with twice as many particles and the reduced search region.

The implementation of importance sampling eliminates the need to run individual simulations over the entire parameter space. It also results in smooth curves that can be modeled with paraboloidal fits. As a result, the new program has a time-to-solution of about five minutes, a reduction by a factor of 25. It also determines a 95% confidence region for the scattering parameters at essentially zero computational cost. The significantly reduced computation time could allow for wide use by experimentalists who are sensitive to time-to-solution.

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**Title of Talk:** Investigation of Multilayers for Magnetic Thermometry using Micro-Magnetic Computer Simulations

**Abstract:**

In the science of temperature measurement, no reliable method exists for measuring temperature variations throughout a volume. A possible solution to this problem, the monitoring of a change in magnetic behavior of bi-magnetic nanoparticles, requires the development of new material systems which have a strong dependence of magnetic behavior on temperature. This study tests the viability of collectively utilizing iron and gadolinium nanoparticles as sensitive thermometers for monitoring small regions. This set of testing was run using a magnetic modeling software known as the Object Oriented Micro-Magnetic Framework (OOMMF) to simulate the change in magnetization ($M$) of iron and gadolinium multi-layer thin films with a change in applied magnetic field ($H$).

Within OOMMF, we determined the optimal parameters for efficient simulation of the magnetization of 4 mm x 4 mm samples of various single-layer and multilayer thin films. To show this, the simulation size of 4 $\mu$m x 4 $\mu$m sufficiently represented the actual measured sample due to a convergence of the $M$ vs. $H$ curves on a single set of points. A decrease in the simulation unit cell thickness showed a non-converging increase in the saturation magnetization of the sample. For the multilayer samples that were simulated, the negative interface exchange interaction between the layers produced a flatter S-shape in the $M$ vs. $H$ curves. Additional tests include comparing the $M$ vs. $H$ curves determined from simulations with $M$ vs. $H$ curves measured experimentally, adjusting the initial conditions of the simulations based on the results of the experimental data, and observing the changes in the $M$ vs. $H$ curves when the temperature of the system is adjusted. The simulation conditions and observations obtained in our study will identify configurations that might be viable for fabricating additional thin films and nanoparticles with strongly temperature-dependent magnetization. The temperature dependence of this type of system will provide avenues for advances in high sensitivity temperature measurement and imaging.
Title of Talk: Organic Transistors: Measuring Changes in Device Current using SAMs to Modify Work Function and Dipole Moment of the Contact Surface

Abstract:

Organic semiconductors have the potential to contribute to the growing fields of flexible and bio-compatible electronics due to their ease of fabrication, flexibility, and chemical tunability. One highly anticipated device application is organic based transistors, the building blocks for state-of-the-art electronic systems. However, the lack of understanding of charge transport in organic semiconductors limits the ability to create high performing devices. One issue lies at the interface between the organic semiconductor and the metal electrode where there exists a difference between the metal work function and the organic’s highest occupied molecular orbital (HOMO) or lowest unoccupied molecular orbital (LUMO) level. This energy level difference creates an energy barrier which impedes efficient charge injection. Self-assembled monolayers (SAM) of organic molecules are known to remediate this issue by generating an interface dipole at the metal/organic interface causing a vacuum energy level shift, therefore modifying the metal work function. The goal of this project is to assess device performance in organic field effect transistors (OFET) using single crystal rubrene by tuning the metal work function of the source and drain electrodes with a newly developed set of selectively fluorinated SAMs. The fluorinated SAMs were compared against other widely used monolayers to isolate and understand the impacts of the changing work function. Contact angle and UPS/XPS measurements were used to measure the quality of the SAMs prepared, and transistor devices were made on the modified gold to measure the impact on I-V characteristics.

Title of Talk: Progress using Laser Interferometry to Determine Radiation Dose

Abstract:

Absorbed dose is the measure of how much energy is deposited into an amount of matter per unit mass by ionizing radiation. Dosimetry of medical radiotherapy beams in the US is traceable to the NIST standard water calorimeter, which uses thermistors and lock-in detection to achieve microKelvin sensitivity. In an effort to produce a more flexible standard suitable for calibrating dosimeters used in quality assurance of modulated and particle-beam therapies, the NIST Dosimetry Group is exploring the use of laser interferometry as a basis for absolute dosimetry. Absorbed dose is determined based on the temperature induced changes in the index of refraction of an irradiated phantom placed in one of the paths of the split beam. Preliminary investigations have been carried out by SURF and SHIP predecessors using prototype Michelson and Mach-Zehnder interferometers to demonstrate suitability of the technique for detecting heating by radiotherapy beams. To assess detection sensitivity of the interferometer and diagnose sources of noise, we are developing automated test cells which can be used to vary optical path length (phase) at prescribed levels with sufficient high precision to mimic the effects microKelvin changes would produce on a typical water phantom. Controls and measurement capabilities are being consolidated and put into LabVIEW to make easy-to-use virtual interfaces to run the experiment and make analyses. A design involving Peltier coolers is further being evaluated for use with nano-scale devices undergoing radiation hardness testing for a NIST-on-a-Chip project related to photonic dosimetry.
SURF Student Colloquium
NIST – Gaithersburg, MD
August 1-3, 2017

Name: Christian Zaytoun
Grant Number: 70NANB16H067

Academic Institution: Carleton College
Major: Statistics

Future Plans (School/Career): Graduate School for Applied Statistics

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Engineering Physics Division

NST Research Advisor: Xiaoyu Alan Zheng

Title of Talk: Beretta 96G Persistence Study in Firearm Identification

Abstract:

The purpose behind the Forensic Toolmark Analysis Project (FTAP) is to give firearms examiners the ability to have more objective conclusions in their work. Historically, a firearms examiner would search for matching marks on a bullet or cartridge case using a comparison microscope. Any seasoned examiner knows that there are multiple regions of interest on bullets and cartridge cases in which a firearm leaves its unique toolmarks. These microscopic marks are exactly what FTAP focuses on to quantify similarities.

Ten thousand shots were taken from three Beretta 96G firearms to simulate the lifespan of the gun. Of the ten thousand rounds, sixty-three sets of cartridge cases and bullets were collected, three at every five hundredth firing. By scanning both the breach face and the firing pin of each cartridge case and running correlations amongst those scans, we plan on discerning whether a cartridge case is identifiable from shot 1 to shot 10,000 of a Beretta 96G. We also hope to find whether or not there are any aggregate similarities in the unique signature a Beretta 96G firearm leaves on a cartridge case.

Name: Peter Zhou
Grant Number: 70NANB16H164

Academic Institution: University of Maryland, College Park
Major: Physics

Future Plans (School/Career): Graduate school

NST Laboratory, Division, and Group: Physical Measurement Laboratory (PML)

NST Research Advisor: Ian Spielman

Title of Talk: Bragg diffraction as a probe of transition to a Bose-Einstein condensate

Abstract:

Bragg scattering is a powerful tool for probing the properties of periodic structures. Originally used in x-ray diffraction crystallography, Bragg scattering has become a widely used technique in atomic physics for studying ultracold atoms bound in periodic optical potentials.

First, an apparatus was constructed to examine the Bragg scattering of light on a diffraction grating. The geometry of the grating is analogous to the atomic distribution in a one-dimensional lattice, and therefore serves as a useful model for Bragg scattering on ultracold atomic systems.

The diffraction efficiencies of blazed and holographic gratings were measured as a function of the incident angle and polarization of a 779 nm laser beam. The zero and first-order diffracted beams were also observed and their dependence on the incident angle was found to be consistent with the general diffraction grating equation.

The second major component of this project was to examine the Bragg-reflected light off of Rubidium 87 atoms undergoing a phase transition to Bose-Einstein condensation. These measurements were performed by taking fluorescence images of the atoms, which were compared with the time-of-flight absorption imaging without the optical lattice confinement. Across the phase transition, any correlation length satisfying the Bragg condition will result in the increase of the Bragg signal.
Liddle, Anna - TPO
Reilly, Erin - SCO
Resnick, Benjamin - TPO
### Name: Anna Liddle

**Grant Number:** 70NANB16H

**Academic Institution:** University of Maryland, College Park

**Major:** Neurobiology & Physiology, Dance

**Academic Standing (Sept. '17):** Sophomore

**Future Plans (School/Career):** Pursuing a PhD in neuroscience.

**NIST Laboratory, Division, and Group:** Technology Partnerships Office, Division 401

**NIST Research Advisor:** Paul Zieliński, Jack Pevenstein

**Title of Talk:** Dance Therapy and Rehabilitative Medicine

**Abstract:**

There is a growing need for research in rehabilitative medicine. Our troops, cancer patients, trauma survivors, and elderly, along with any other category of human beings one could think of, need it to improve their health and quality of life. By speaking to researchers and clinicians, as well as performing thorough literature searches, giving a workshop to middle school girls, and writing a paper, I have gained insight into the field of rehabilitative medicine. Rehabilitative medicine includes any treatment that will help alleviate symptoms and resolve issues that present themselves in someone who has experienced some sort of medical problem, most commonly a chronic illness/condition or trauma – something not easily fixed by prescribing antibiotics or bedrest, or prevented by diet, exercise, and vaccines. I explored many aspects of the field, but most deeply investigated dance therapy and its potential to mitigate the effects of many conditions. I found that dance therapy can be used to effectively diminish symptoms of Parkinson’s, dementia/Alzheimer’s, the psychological effects of cancer, depression, heart conditions, trauma, schizophrenia, autism, and stroke. The growing interest in dance therapy and rehabilitative medicine, and the number of promising results, reinforces the belief that this field is well worth investigating and has the potential to improve millions of lives.

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### Name: Erin Reilly

**Grant Number:** 70NANB16H

**Academic Institution:** University of Maryland, College Park

**Major:** Bioengineering

**Academic Standing (Sept. '17):** Sophomore

**Future Plans (School/Career):** Graduate School for a Master’s Degree in bioengineering

**NIST Laboratory, Division, and Group:** Special Programs, Standards Coordination Office (SCO) and Material Measurements Laboratory (MML) Biosystems and Biomaterials Division

**NIST Research Advisor:** Clare Allocca (SCO), Sumona Sarkar (MML) and Laura Pierce (MML)

**Title of Talk:** Making Standards Count: Terminology and Analytical Methods for Biotechnology Standards

**Abstract:**

The International Organization for Standardization (ISO) established Technical Committee (TC) 276 to develop standards for biotechnology to enable more reliable, higher quality, and better understood globally competitive products. My project contributes to the development of ISO/TC 276 standards via two of its Working Groups (WGs) – Terminology and Analytical Methods. An inventory of biotechnology-related terms is being developed in the Terminology WG as a resource for working group experts, academic researchers, and others to use as a basis for common understanding of biotechnology-related terminology. As a Technical Report, this inventory of terms must undergo a consensus-generating process before being accepted as a globally recognized document. My work involved producing the U.S. response to this document before its final stages. I reviewed the terms and their definitions for clarity, relevance, and credibility, and ensured that each term was searched within a minimum set of credible and relevant sources (e.g., ISO, International Vocabulary of Metrology (VIM), British Standards Institution (BSI), U.S. Food and Drug Administration (FDA)). I assembled comments from U.S. experts into the official ISO commenting template for submission to the Terminology WG.

I also contributed to the Analytical Methods WG in the area of cell counting, which is a fundamental measurement in biotechnology. The Analytical Methods WG is currently developing an ISO Standard on methods to evaluate the quality of cell counting methods. A major source of variability that may affect the quality of imaging-based cell counting methods is the image analysis step of the measurement process. Using the experimental design and statistical analysis methods outlined in the ISO cell counting standard, I evaluated a series of cell counting measurement processes that utilize different image analysis settings. I established these settings by evaluating a range of cell samples with varying morphologies and levels of viability. Results suggest that the quality of the cell counting method is affected by the image analysis settings, so I developed systematic strategies for establishing appropriate image analysis settings to improve user confidence in the automated cell counters. These studies will support further development of use cases for the cell counting standard currently under development in ISO/TC 276.
Abstract:

Every day, NIST scientists are working hard to advance measurement science, standards, and technology in a meaningful way. While this technology can be very beneficial to the American people, it is often difficult to provide the public access to this technology. It is critical that the American people can reap the benefits of the hard work of the NIST scientist. One way NIST is able to get the technology they develop to industry is by licensing the technology to the private sector and allowing them to incorporate the NIST's inventions with their products. NIST scientists can also engage in a Cooperative Research And Development Agreement (CRADA) with public businesses to share ideas and work toward creating ideas and products which will help the American people.

To assist in the marketing and licensing of NIST and other federal laboratory technology, I worked to create a workshop in association with Maryland TEDCO and Montgomery County Economic Development Corporation on the topic of smart cities. The workshop would include NIST scientists and other federal lab researchers, university researchers, local businesses and entrepreneurs, and government officials. The goal of this event is to develop an integrated planning framework for addressing the application of smart cities technology to problems in the areas of public transportation, public safety, health services, energy, water, and agriculture. In order to create this workshop, I researched, analyzed, and summarized smart city and Internet of Things technology for technical and non-technical audiences to inform workshop content and discussion. I accomplished this by sitting down with scientists at NIST across many fields and disciplines and analyzed their work and determined if their research could be beneficial to the workshop.

The workshop will take place on September 12th at NIST in the heritage room.
Post-doc Association (PEAR) Panel Discussion:

Graduate School (application process, funding, standardized testing, selecting an institution/mentor and more)
SURF students in NanoFab Lab
STEM on the Hill Day
Capitol Hill visit
Women in STEM (WiSTEM) Meal with a mentor
STUDENTS

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<td>Xinyu</td>
<td>City University of New York City College</td>
<td>Access Control Rule Logic Circuit Simulation (ACRLCS)</td>
<td>ITL</td>
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<tr>
<td>Zaytoun</td>
<td>Christian</td>
<td>Carleton College</td>
<td>Berretta 96G Persistence Study in Firearm Identification</td>
<td>PML-PL</td>
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<tr>
<td>Zhou</td>
<td>Peter</td>
<td>University of Maryland College Park</td>
<td>Bragg diffraction as a probe of transition to a Bose-Einstein condensate</td>
<td>PML-PL</td>
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