SURF

Summer Undergraduate Research Fellowship

Colloquium 2018

Greetings!

On behalf of the Director's Office, it is my pleasure to welcome you to 2018 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, #2018SURFColloquium.

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)

Organizational Unit (OU)	Name
Director's Office	Brandi Toliver, Managing SURF Program Director
Director's Office	Kara Arnold
Center for Nanoscale Science and Technology	Kartik Srinivasan
Engineering Lab	Lisa Jean Fronczek
Engineering Lab	Cartier Murrill
Engineering Lab	Stephen Potts
Information Technology Lab	Lotfi Benmohamed
Information Technology Lab	Michaela Iorga
Information Technology Lab	Elizabeth Lennon
Information Technology Lab	Derek Juba
Communications Technology Lab	David Griffith
Material Measurement Lab	Andre Striegel
Material Measurement Lab	Amanda Forster
NIST Center for Neutron Research	Julie Borchers
NIST Center for Neutron Research	Joseph Dura
Physical Measurement Lab-Electrical Eng	Joseph Kopanski
Physical Measurement Lab-Electrical Eng	Richard Steiner
Physical Measurement Lab-Electrical Eng	Darwin Reyes-Hernandez
Physical Measurement Lab-Physics Lab	Cameron Miller
Physical Measurement Lab-Physics Lab	Uwe Arp
Physical Measurement Lab-Physics Lab	Maritoni Litorja
Technology Partnership Office	Paul Zielinski
Standards Coordination Office	Nathalie Rioux

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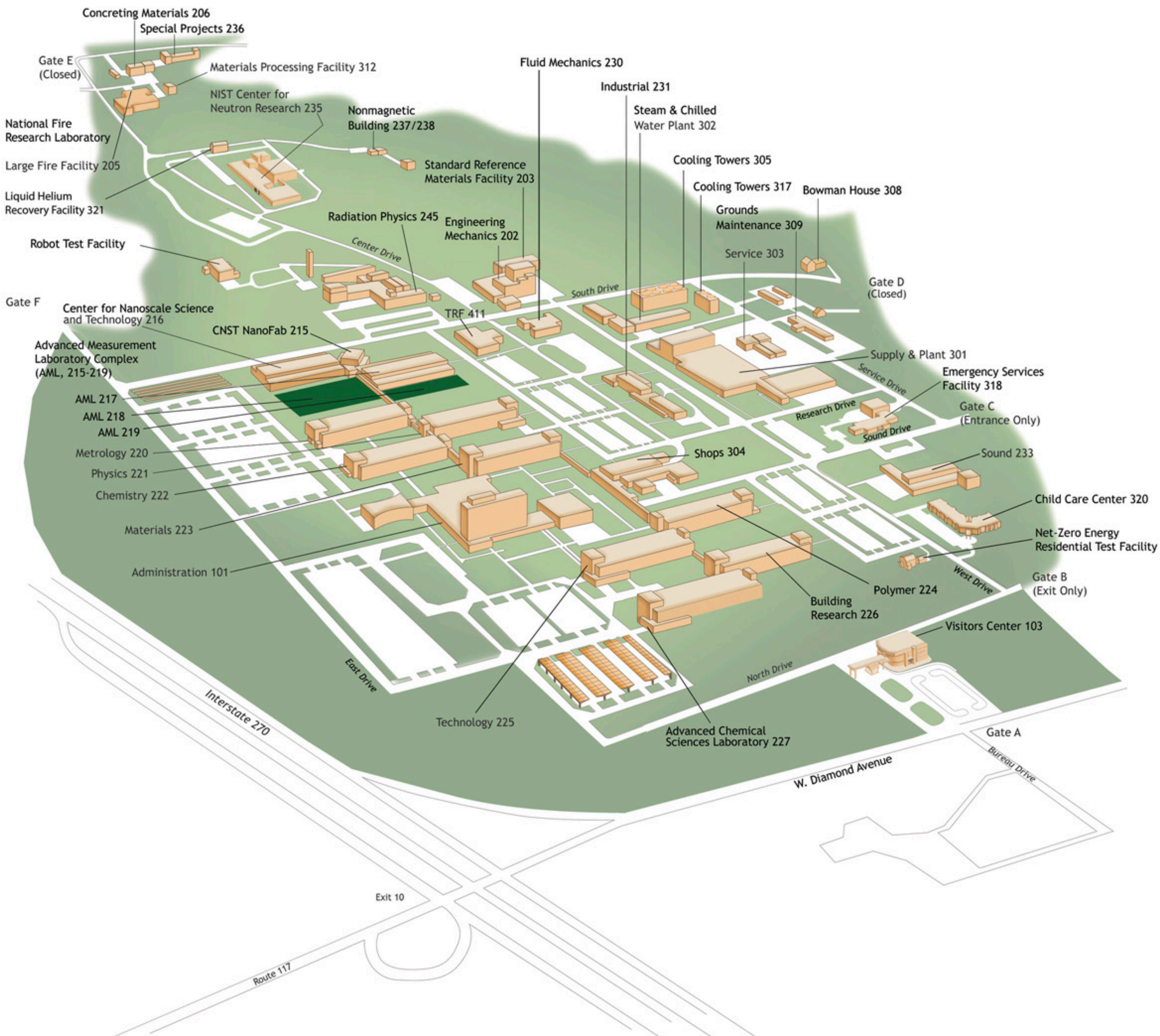
Campus Map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SURF Colloquium Plenary Session (Admin 101 Building/Green Auditorium)

Time	Agenda
9:00A	**Welcome**
	Session Moderator: TBA
9:15A	**CNST** *Thomas Marsh* : Solving the Shortest Path Optimization Problem using a
9:40A	**CTL** *Morgan Warner* : Stop Interrupting Me(ssages)
10:05A	**EL** *Lela Bones: Visualizing and Synthesizing Data from Maintenance Logs for Smart Manufacturing Analysis*
10:30A	Break
10:45A	**ITL** *Naveen Shankar* : Using the Arduino for True Random Number Generation
11:10A	**MML** *Elena Musteata:* Synthetic Biology for Living Sensors: Characterizing Fitness Landscapes of Engineered Genetic
11:35A	**NCNR** *Paul Neves:* All Tied Up in Knots: Skyrmions in Chemically Substituted Cu2OSeO3
12:00P	**PML** *Alex Sredenschek* : Silicon Surface Functionalization for Battery
12:25P	**Special Programs** *Alexsandra Corrigan:* A Cell-ing point for Standards: Terminology and Analytical Methods for Biotechnology Standards

SURF Colloquium Parallel Session: Tuesday August 7, 2018 (Afternoon)

	Lecture Room A	Lecture Room B	West Square	Heritage Room	Lecture Room D
	MML/NCNR_ChemBio	MML/NCNR_MatSci	ITL	EL	PML_PL
Time	Moderator: Dr.Andre Striegel	Moderator: Dr. Jeanita Pritchett	Moderator: Michaela Iorga	Moderator	Moderator: Daniel Hussey
2:20P	*Tiffany Cao* :Characterization of electronic cigarette aerosol on hard surfaces	*Alexis Brake:* Ultrasound for materials research: Developing methods to quantify internal displacements in soft material tissue phantoms	*Matthew Kupferschmid* : Understanding P@$$w0rds – password rule comprehension vs password generation	*Timothy Kim* : Solar Microgrid Performance and Optimization	Zachary Whiting: Graphite Calorimetry with a Mach-Zehnder Interferometer
2:40P	*Zachary Clifford:* Physical and Chemical Transformation of Silver Nanomaterial Containing Textiles After Use and Disposal	*Faraz Burni:* Ageing of Poly(*p* -phenylene terephthalamide) Fibers Used in Soft-Body Armor	*Sophia Abraham* : Authentication of RFID Communication with Wireless Identification and Sensing Platform (WISP)	*Abhinav Pandey* : A Digital-twin of an IEEE 1451 Smart Temperature Sensor for CPS/IoT Research	*Rhett Croley:* Data Analysis of Alpha-Gamma Neutron Monitor Technique
3:00P	*Shakira Gonzalez:* Characterization of Fluorescent Dyes for the Assignment of Fluorescence Intensity to Calibration Microspheres for Flow Cytometry	*Patrick Ott:* Structure-property relationships in multi-functional hierarchical fiber nanocomposites	*Xinyu Xiong* : Z Model for Next Generation Access Control (NGAC) Mechanism	*Alejandra Lopez Moralez* : Data Collection and Management for Critical Buildings to Support the Investigation of Hurricane Maria's Effect on Puerto Rico	*David Mullins:* Neutron Bragg Edge Imaging
3:20P	*Brianna Higgins:* Design and synthesis of mechano- responsive fluorophores for localized visualization of damage in polymer composites	*Sejal Shah:* Rheology of shear thickening fluids		*Angel Miranda* : Infrastructure Support of Critical Buildings	*Alexander Todd: Far* Field Neutron Interferometry
3:40P	*Julianna Koehl:* Optimization of Ring Expansion Cationic Polymerization as a Route to Ideal Networks	*Hallie Miller:* Illuminating the transparency of glass elemental composition	*Arsen Klyuev* : Using Block Matrices to Provide Erasure Capabilities to Blockchains Without Losing Integrity	*Harrison Kraus* : Analysis of Garage Door Failures and Subsequent Effects on Residential Building Performance during the May 22, 2011 Tornado in Joplin, MO	*Sai Meghasena Chavali*: Systematics in the Neutron Lifetime Measurement
4:00P	*Claire Sturek:* Antimicrobial Properties of Novel Class V Restoratives	*Julia Trowbridge:* Improving the light extraction efficiency of zinc oxide nanofin LEDs	*Richard Williams* : Automatic Verification of Cryptographic Algorithms using SAW	*Timothy McIntyre* : Analysis of Damage Parameters and Degree of Damage Variability in Residential Building Performance from the 2011 Joplin Tornado	*Peter Orban:* Ionization Chamber Response Dependence on Amb ient Environmental Conditions
4:20P	*Ha Tran* : Identification and Quantification of Allergenic Milk Proteins in Food	*Keshav Bhatnagar:* Developing Operation Procedures for the Meca500 to Autonomously Swap Powder Samples in Divergent and Parallel Beam Diffractometers (DBD and PBD).	*Sydney Pugh* : Developing Effective Test Strategies for Cryptographic Algorithm Implementations	*Andrew Seamone* : Structural Testing of Enhanced Steel Gravity Connections for the Mitigation of Disproportionate Collapse	*Francis Walz:* An active LCR circuit for cooling highly charged ions captured in an ion trap
4:40P		*Michael Hamati:* Synthesis and Characterization of Monodisperse Cerium Oxide Nanomaterials	*Samantha Halam* : Analyzing Cybersecurity in Academia Regarding the Botnet Report		*Gabriel Alberts*: PrediCTing Errors: Test Method Development for CT Systems

SURF Colloquium Parallel Session: Wednesday August 8, 2018 (Morning)

	Lecture Room A	Lecture Room B	West Square	Heritage Room	Portrait Room
	MML/NCNR_ChemBio	**MML/NCNR_MatSci**	**ITL**	**EL**	**PML_PL**
	Moderator: Dr. Ashley Beasley Green	Dr. Guebre Tessema, NSF	Moderator: John Schlueter	Moderator	Moderator: Uwe Arp
9:00A	*Jack Blitz:* Droplet Digital PCR Assay Development of Clinical Reference Material for Epstein Barr Virus DNA	*Samantha Isaac* : Monte-Carlo Exploration of Focused Neutron Guide Geometries	*Jesse Zhu* : Use of lightfield cameras for capturing footwear impression: best practice and comparison	*Rushad Antia* : localhost:3000/robotmonitor.html – Integrated Robot Monitoring System	*Michael Doris*: Encoding Arbitrary Phase and Amplitude Modes on Laser Light with A Digital Micro-Mirror Device
9:20A	*Sulan Wu:* Standardization of HER2 gene copy number variation measurements in liquid biopsy by digital PCR	*Hannah Burrall* : Optimization of 3He neutron spin filters for the neutron spin echo spectrometer	*Paul Steves* : Augmented Reality Systems and Associated Metrics and Analytics	*Nickolas Eusman* : Railroad grade crossing simulator for use in cybersecurity testbed	*Benjamin Eckardt*: Increasing Efficiency of Temperature Controllers in the Laboratory
9:40A	*Adam Broerman:* A Computational Workflow for Annotating LC-MS Metabolomics Data from Biomanufacturing Cell Cultures	*Nathaniel Kaneshige* : Simulation of prompt gamma emission tomography by Compton scattering and the implementation of a neutron tomography system	*Paul Armstrong* : Virtual Reality as a tool for Cell Microscopy	*Brian Galfond* : Measuring and Diagnosing Machine Tool Errors Using an Inertial Measurement Unit and Inductive Proximity Sensors	*Jacob Siegel:* Constructing a Primary Vacuum Standard using Bitter Electromagnets
10:00A	*Candace Young:* Development of Metabolomics Quality Control Materials for Precision Medicine and Strategies for Forensic Hair Analysis	*Ryan Underwood* : Determination of crystallite orientation distribution function (ODF) from neutron diffraction data	*Joseph Waysack* : Monitoring Super Computer Simulations	*Meir Kreitman* : Characterization of Single Scan Laser Tracks on Nickel Super Alloy 625 Using Nanoindentation	*Dylan Kirsch:* Raman Spectroscopy of Tin-based Intermetallic Thin-Film Libraries for Next Generation Rechargeable Battery Anodes
10:20A	*Sabrina Martin:* Drop-On-Demand Inkjet Printing for Preparation of Oral Drug Delivery Films	*Abigail Wilson* : Applying Reinforcement Learning to the Determination of Crystal Structures with Neutron Diffraction	*James Biggins* : Virtual Tours: Experiments in Monoscopic and Stereoscopic Virtual Reality	*James Arnold* : Creating a Database for Designing Energy Efficient Houses	*Stephen Meek*: An improved method to measure very low fluid flow rates for diagnostic medical and biotechnology applications
10:40A			Break		
	Moderator: Dr. Christine Bergonzo	Dr. Leonard Spinu, NSF	Moderator: Ryan Evans	Moderator	Moderator: David Allen
11:00A	*Kunal Dharmadhikari* : Structural Basis of ClpS Specificity Probed by Molecular Dynamics Simulations	*Joshua Devorkin* : Cellulose under pressure for new biopolymers	*Qing-Hai Li* : Analysis of Microfluidic Flow Rate Measurements	*Marco Capraro* : Data Management Strategy	*James McLaurin*: Investigation of substrate suitability for focused helium ion beam machined nanofluidic structures
11:20A	*Elijah Williams:* Improving the Measurement Quality of Hydrogen Deuterium Exchange Mass Spectrometry	*Zachary Riedel* : Capillary µRheoSANS for High Shear Rate, Low Volume Studies	*Felix Perez* : Facilitating Development of Alternatives to Monoclonal Antibodies Through Readily accessible Web Application Services	*Jonathan Garner* : Advanced Sensing Development to Support Robot System Prognostics and Health Management	*Eileen Stauffer*: Evaluation of FPGA-Based Laser Stabilization
11:40A	*Allison Horenberg:* Cell Viability in Tissue Engineering Scaffolds	*Alexa Cano* : Phase Behavior and Morphology of Microemulsions in a Polymer-Surfactant System	*Kevin Zong* : Software for Single Photon Counter Interfacing and Data Analysis	*Peter Mnev* : Analyzing Agility of Robot Systems through Simulation	*Hunter Wages*: Using Magnetic Field Inversion to Produce Current Density and Magnetization Distribution Images
12:00N	*William Jones:* Assessments and quantification of mineralization in dental pulp microtissues by phase imaging	*Caleb Wigham* : Crosslinking silica-based nanoporous networks under ambient conditions	*Henry Schmale* : Benchmarking Numerical Approaches for Solving the Time-Dependent Schrodinger Equation in One Dimension	*Esteban Segarra* : Integration of Wearable Sensors into Virtual Reality and Augmented Reality Interfaces for Human-Robot Interaction	*Galahad Wernsing: Real Time Data Analysis and Phase Correction for Optical 2D Spectroscopy*
12:20P	*Grace Henry*: Purification of Chorismate Mutase from M. tuberculosis for Novel Inhibitor Evaluation	*Krista Balto* : The Conformation of a Hydrophilic Di-block Copolymer on Silica	*John Nolan* : Compositional Approaches to Power Flow Problems	*Xiang Li* : Predictive Modeling of Collaborative Robot Interactions	*Wiley Hundertmark*: Using Optical Methods to Investigate Productivity and Carbon Fluxes in Urban Forests
12:40P			Lunch		

SURF Colloquium Parallel Session: Wednesday August 8, 2018 (Afternoon)

	Lecture Room A	Lecture Room B	West Square	Heritage Room	Portrait Room
	MML/NCNR_MatSci A	**MML/NCNR_MatSci B**	**ITL**	**EL**	**PML-Electrical Eng**
	Moderator: Prof. Mohamad Al-Sheikhly	Dr. Engin Serpersu, NSF	Moderator: Derek Juba	Moderator	Moderator: Richard Steiner
1:30P	*Rachel Orenstein:* Building a resource registry and data repository for High-Throughput (Combinatorial) Experimental materials research	*Temiloluwa Okusolubo* : Correlating Gramicidin Ion-Channel Formation to Artificial Membrane Dynamics	*Varsha Vejalla* : Measuring Climate Change using Ice Cores	*Frederick Norwood* : Measurement and Tuning of Motorized-Dynamic Bending and Calibration Machine to Test Disposable Human-Collaboration-Robotics Safety Artifacts	*Laurelia May-Pohlman*: An Improved Reference for Spectrograph Calibration at Low-to-Moderate Resolutions
1:50P	*Ryan Smith:* Predicting the Elastic Properties of Metallic Glasses with Machine Learning	*Emily Blick* : Exploring the rheological properties of dense lipid vesicle solutions as models for liposomal nanomedicines	*Golda-Meir Chiong* : Computational Reproducibility	*Omar Aboul-Enein* : Performance Measurement of a Manipulator-on-a-Cart	*Merrik Malin*: High Speed Control Circuit for Single Photon Avalanche Detection
2:10P	*James Riet:* An Evaluation of Polymer Encapsulation as a Means of Minimizing the Degradation of TNT for Explosive Trace Detectors	*Carrie Stemple* : Characterizing Adjuvant-Protein Interactions During Freeze-Thaw Cycles	*David Miller* : Stochastic Modeling of Round-off Errors in Scientific Computing	*Katrina Carlin* : Accelerated Weathering of Graphene-Polymer Nanocomposites	*Jeffrey Borres*: Robotics mass exchange for advanced metrology
2:30P	*MaKayla Turner:* Interaction of Water with Titanium Oxide Surfaces: A Theoretical Study	*Gregory Suczewski* : Incorporation of the Beta Approximation in SASView	*Alejandro Vega* : The HTGS Generator: A Tool for Generating Code for Multi-core systems	*Samuel de Oliveira* : Degradation of Field-Exposed Photovoltaic Backsheets	*Vaishnavi Murthy: Environmental Monitoring and Control for Metrological Applications*
2:50P	*Steven Hall:* Charge Expanded Ensemble for Efficient Sampling of Ionic Systems		*Aidan Malanowski* : Combining syntactic parsing and vector semantics for keyphrase extraction for the root- and rule-based method	*Joshua Hubbard* : Essential Work of Fracture and Digital Image Correlation Analysis of Crack Propagation in PET after Accelerated Weathering	Sumaiyah Sarwat: Watt-Hour Meter Testing
3:10P			Break		
	CNST	**MML/NCNR_MatSci**	**ITL**	**EL**	**PML-Electrical Eng**
	Moderator: *Liya Yu*	Moderator: Dr. Charles Ying	Moderator: Lotfi Benmohamed	Moderator	Moderator: Maritoni Litorja
3:20P	*Emma Rogers* : The Role of Directional Shear Flow in the Inflammatory Response of Endothelial Cells	*Katie Behnert* : Physical Components of Secondary Pump Condition-based Monitoring System	*Nicholas Nachega: A Test Transport Layer Security (TLS) Server for the DNSSEC Authentication Chain Extension*	*Trinny Lai* : Analysis of Automotive Paints under Weathering Conditions	Gabriela Arp: Spectral Analysis of Glycated Hemoglobin
3:40P	*Shannon Jin* : Study of DNA Origami Under Shear Conditions	*Abdullah Weiss* : Digitization of a Secondary Pump Condition-based Monitoring System	*Surafel Hailu* : NDN-based IoT prototype deployment by using the ESP32 and Raspberry Pi platforms	*Christopher Littrell* : Analysis of the Degradation of Polymeric Components Used in Photovoltaic (PV) Systemsn	*Alana Dee*: Comparison of Current Detection Methods in the 3rd Generation Dual Source Bridge for DC Resistance Measurements
4:00P	*Holland Rhodd-Lee* : A New Approach to Measuring Neuronal Differentiation in P19 Embryonal Carcinoma Stem Cells	*Omar Cavazos* : NBSR Thermodynamic Performance Analysis		*Vanda Luu* : Key Parameters Effecting Polyester Weathering	*Kevin Ho:* Development of Microgrid Simulation System for Hardware-in-the-Loop Study of Power Grid Monitoring and Control
4:20P		*Kirill Stakhovsky* : Operating a Virtual Nuclear Reactor using HoloLens Technology		*Christopher Carangelo* : Development of Cement 3 D Printing Test Artifact	*Isabel Damazo:* Developing a Method for Measuring Intracellular Calcium Concentrations
4:40P		*Aubrie Weyhmiller* : Online Platform for Radiological Computations		*Pablo Dean* : Mineralogical Phase Analysis of Portland Cement by X-ray Diffraction and Scanning Electron Microscopy	*Mathew Fu*: A Virtual Kelvin Probe Microscope
5:00P			End		

SURF Colloquium Parallel Session: Thursday August 9, 2018 (Morning)

	Lecture Room A	Lecture Room B	West Square	Heritage Room	Portrait Room
	CNST	**MML/NCNR_MatSci**	**ITL**	**EL**	**PML-Electrical Eng**
	Moderator: *Liya Yu*	Moderator: Dr. Jonathan Seppala	Moderator	Moderator	Moderator:
9:00A	*Erik Isele* : All-dielectric Terahertz Metasurfaces: Fabrication and Characterization	*Rachel Devers:* The development of an electron microscopy dossier		*Ann Collins* : Community Resilience	
9:20A	*Devin Jessup* : Simulating Magnetic Skyrmion-Skyrmion Interactions	*Simin Manasiya:* Polyelectrolyte stiffness in different salt concentrations and salt types		*Michael Bichnevicius* :Evaluation of a CO2 Ground-Source Air Conditioner	
9:40A	*Hengming Li* : Process Development for Area-Selective Atomic Layer Deposition using a Novel Photoresist	*Ethan Finlay:* Exploring Clinically Relevant Approaches to Reduce Polymerization Stress of Dental Composites		*John Walsh* : Measuring Performance of an Airflow-Optimized Condensing Unit	
10:00A	*Stephen Tovcimak Jr.* :Fabrication and Characterization of the Surface and Interfacial Effects on the Directed Self-Assembly of Block Copolymers (BCPs)	*Klara Keim:* Development of Microfluidic Platforms Recapitulating Oral Microvasculature		*Justin Sorra* : Laboratory Validation of HVAC-Cx Building Commissioning Software	
10:20A				*Jennifer Bergeson* : Powering the Internet of Things: Harvesting Ambient Energy with Photovoltaics	
10:40A		Break			
	MML/NCNR MatSci A	**MML/NCNR_MatSci B**	**CTL**	**EL**	**Special Programs**
	Moderator: Dr. Brandi Toliver	Moderator: Dr. Wyatt Vreeland	Moderator: David Griffith	Moderator	Moderator:
11:00A	*Sally Jiao:* Determining Protein and Polymer Stability through Thermodynamic Extrapolation and Active Learning	*Eric Anderson:* ROMP Bottle Brush Polymer Structure Characterization via NMR and Computational Methods	*Hiwot Gezahegn* : Analysis and Validation of Mission-Critical Push-To-Talk (MCPTT)	*Patrick Feeney* : Automated Translation of MATLAB Programs to Python to Increase Accessibility and Cross-Platform Compatibility of Open Source Software	*Candice Ionescu*: China's Changing Standards Infrastructure: A New Approach to the Global Stage
11:20A	*Kamryn Kant:* Computing Thermodynamic Properties of Fluids Confined in Nanoporous Materials with High-throughput Molecular Simulations	*Viviana Rodriguez Cardenas:* Method Development and Depth-Profiling Degradation Measurements of Beach Plastics	*Steven Fan* : Video Streaming Models	*Luis Serrano* : Validation of Fire Dynamics Simulator	*Ángel Jarel Resto García and Yinaris Guzman Cruz* : Advanced Manufacturing & Development and growth of technology-based businesses in Puerto Rico
11:40A	*Julie Yagodich:* Encoding Gas Adsorption Isotherms for Standard Reference Data and Use	*David Yoon:* Measuring Viscosity Through a Microliter Capillary Rheometer	*Zachary Luckabaugh (SHIP)* : A Graphical User Interface for Public Safety Communications Simulations	*Jacob True Furrh* : Hurricane Maria: Reconstructing Flood Hazards through Emergency Messaging	Zachary Taylor: Technology Transfer, Invention Disclosures, and Supporting the MBDA Mission
12:00N	*Shannon Bernier:* Thermochemical analysis of SRM fuel blends using the laser-driven thermal reactor	*Jeremy Filteau:* Mechanism behind rapid protein aggregation by novel azide-assisted chemistry		*William Saar* : Single and Double Fence Flame Spread in the Wildland Urban Interface	
12:20P	*Nicholas Strogen:* The Effects of Chlorine Exposure on the Performance and Morphollogy of Polyamide Membranes	*Alison Kriz:* High-Aspect Ratio Sulfur-MoS2-Carbon Heterostructure Electrode Materials for High-Performance Li-S Batteries: Design and Multiscale Characterization by Advanced Focused Ion and Electron Beam Techniques		*Gregory Fiola* : Calorimetry Reflexes: Characterizing Response Time of Fire Measurements	
12:40P		Lunch			

SURF Colloquium Parallel Session: Thursday August 9, 2018 (Afternoon)

	Lecture Room A	Lecture Room B	Library	Heritage Room	Portrait Room
		MML/NCNR_MatSci	**Various OU's**	**EL**	
		Moderator: Dr. Rebecca Zangmeister	Moderator:	Moderator	
1:30P		*Ryan Zambrotta:* Atomistic Simulations of the Glass Transition in Small-Molecular Organic Glass Formers	*Elijah Peake (ITL)* : Visualization Software to Analyze Password Policies	*Angelo Calvo* : Case studies for model based requirement generation using the VVUQ pattern	
1:50P		*Eli Fastow:* Annealing Temperature and Underlayer Effects on Perpendicular Magnetic Anisotropy Energy of $Co_{20}Fe_{60}B_{20}$/MgO	*Kevin Boby (ITL)* : Automated Segmentation and Classifcation of Concrete Images	*Ryan Fisher* : Testing of the MTConnect - OPC-UA Companion Specification	
2:10P		*Daniel Ng:* Optimizing Additively Manufactured Inconel 625 for Reliable Performance	*Luke Bezn (ITL)* : Launch and Demonstration of the NIST Homogeneity Assessor	*Cesar Tamayo Claro* : Incorporating Unit Manufacturing Process Models into Life Cycle Assessment Workflows	
2:30P		*Charlie Nitschelm:* Mechanical Measurements of Inconel 625 for Dynamic Forming Simulations		*Alexander Lewis* : Ontology Engineering for Interoperable Manufacturing Process Information	
2:50P		*Eli Janzen:* Calphad Assessments of the Co-Re-Ta and Mo-Ti Systems and Practical Application to the Optimization of hBN Crystal Growth		*Michael Roa* : Linking As-Planned and As-Executed Manufacturing Data in Near-Real Time	
3:10P			Break		
		MML/NCNR_MatSci			
	Moderator:	Moderator: Dr. Anthony Kotula	Moderator:	Moderator	
3:20P		*Kevin McCright:* Uncertainty Quantification and Propagation in Carbon Steel Machining		*Xinran Sun* : Mass Customization Activity Modeling and Standards Landscape	
3:40P		*Leah Borgsmiller:* Impedance Photocurrent Device Analysis of Organic Photovoltaics		*Simin Li* : Additive Manufacturing (AM) Bench Data Processing and Integration for the NISTAM Materials Database	
4:00P		*Emily Roe:* Blade-coating as a scalable route to metal oxide field-effect transistor fabrication		*William Brannon* : Development of Automated Data Acquisition of Hydration Reaction in Microstructue	
4:20P		*Galen Vincent:* Process Optimization of Blade-Coated Polymer Blend Thin Film Transistors		*Alexander Brassel* : Demystifying the performance bottleneck in Rich UI Web-based Applications	
4:40P		*Jordan Winetrout:* Predicting Phase Behavior in Organic Photovoltaic Devices			
5:00P			End		

2018 SURF Student Abstracts by OU

(Alphabetical order, Last Name)

"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."

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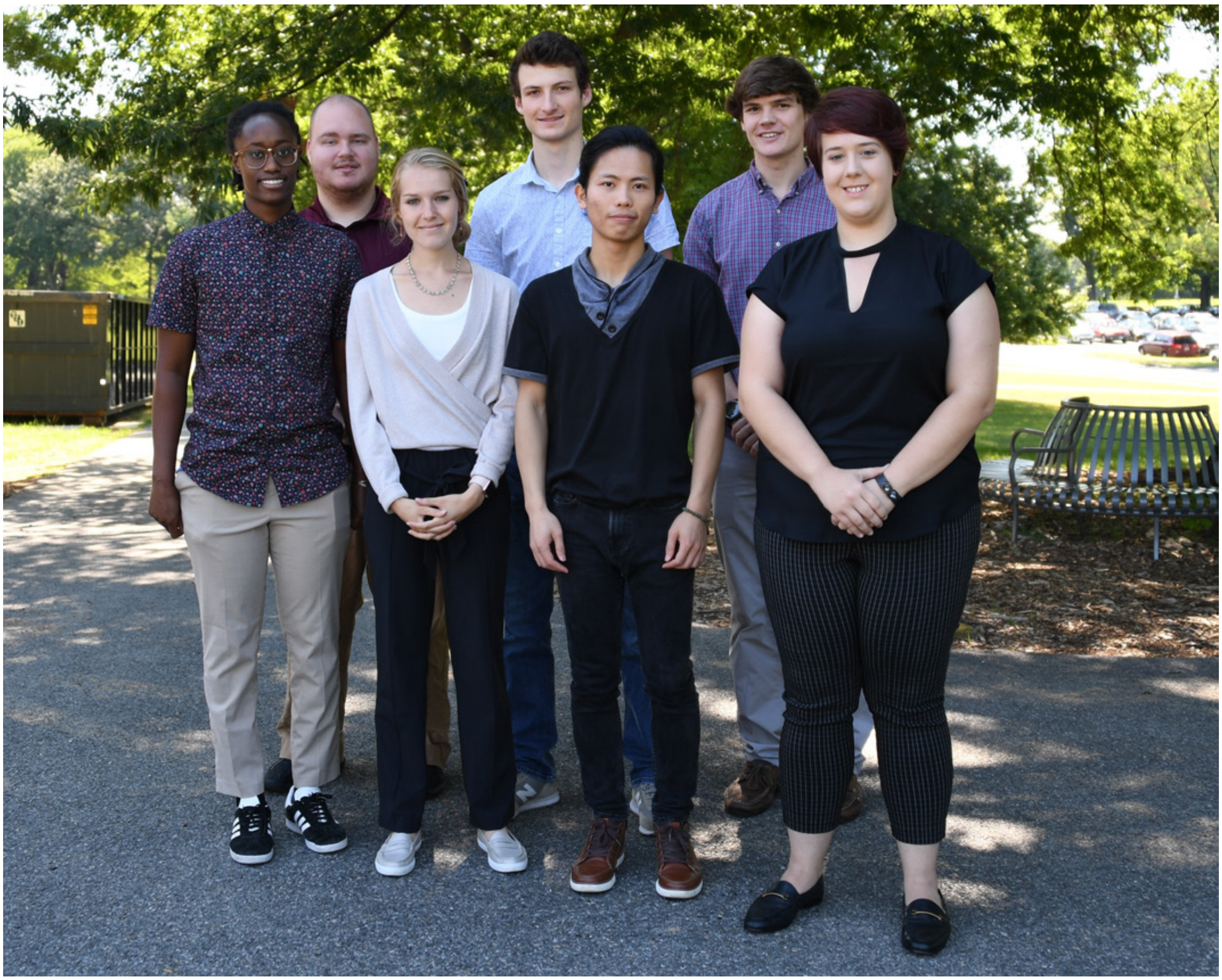


CNST

Last Name	First Name	Lab
Iselle	Erick	CNST
Jessup	Devin	CNST
Jin	Shannon	CNST
Li	Hengming	CNST
Marsh	Thomas	CNST
Rhodd-Lee	Holland	CNST
Rogers	Emma	CNST
Tovcimark Jr	Stephen	CNST

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Erik Isele		**Award Number**	70NANB18H135
Academic Institution:	University of Michigan	**Major:** Engineering Physics	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Technology, Nanoscale Imaging and Spectroscopy Group		
NIST Research Advisor:	Amit Agrawal		
Title of Talk:	All-dielectric Terahertz Metasurfaces: Fabrication and Characterization		

Abstract:
As the need for higher bandwidth telecommunication rises, there is a push into higher frequency communication bands to create room for this demand. One of the regions of interest has been at frequencies that lie within the terahertz (THz) band of the electromagnetic spectrum. While there have been significant developments in the ability to generate and detect THz radiation over the last couple of decades, developing optical components that arbitrarily manipulate the amplitude, phase or polarization of THz waves is still an active area of research. In this paper, we investigate the promise of all-dielectric metasurfaces as high-efficiency, planar optical elements to arbitrarily manipulate terahertz radiation. Metasurfaces are planar array of subwavelength structures that can control the amplitude, phase or polarization of light, allowing for flat devices that can both replace existing diffractive or refractive optical elements, and present novel ways of controlling light. In this project, we spatially characterize the beam-shaping capabilities of metasurfaces, composed of an array of silicon pillars of varying size and geometry, designed to impart arbitrary phase delays and polarizations to the THz wavefront. The devices tested were high numerical aperture lenses and a radial/azimuthal polarizer designed to operate at a frequency of 0.3 THz. We use a tunable continuous wave terahertz spectrometer composed of a custom automated home-built detection system to spatially map the phase and polarization shaping characteristics of the metasurfaces in all three-dimensions with wavelength-scale spatial resolution. The metasurfaces studied here are intended to be used as high-efficiency optical components in a number of applications including, for example, increasing the coupling efficiency to the dominant radially-polarized mode a coaxial-waveguide.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Devin Jessup		**Award Number**	70NANB18H079
Academic Institution:	George Washington University	**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate studies in electrical engineering		
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Technology, Electron Physics Group		
NIST Research Advisor:	Mark Stiles		
Title of Talk:	Simulating Magnetic Skyrmion-Skyrmion Interactions		

Abstract:
Magnetic skyrmions are quasiparticles with nontrivial topology, characterized by localized regions of magnetization reversal. Skyrmions are topologically protected, which means that they are highly stable and resist deformation induced by certain physical forces. In addition, these quasiparticles are small, often less than 100 nm, and are easily manipulated with weak spin-polarized currents. Despite existing studies on single-skyrmion control, multi-skyrmion systems and their associated forces are not well understood. Therefore, the purpose of this project was to develop an understanding of the kinetic interactions between two magnetic skyrmions, using micromagnetic simulations. Utilizing the Object Oriented MicroMagnetic Framework (OOMMF), simulations were developed to explore domain wall movement. Once the motion and control of domain wall movement was understood, these concepts were applied to nucleate skyrmions in magnetic samples. The skyrmions were then manipulated using current-induced spin transfer torques. Larger scale simulations were ultimately performed on the Raritan Linux clusters, and data analysis tools were developed in Python to gather positional information such as centroid location and the radius of individual skyrmions. With all of the data gathered, graphs were produced to track skyrmion movement in multi-skyrmion systems which reveals information regarding the kinetic properties of skyrmion collision.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Shannon Jin		**Award Number**	Click here to enter award number.
Academic Institution: Columbia University		**Major:** Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Pursuing a career in engineering		
NIST Laboratory, Division, and Group:	CNST Nanofabrication Research Group		
NIST Research Advisor:	Jacob Majikes		
Title of Talk:	Study of DNA Origami Under Shear Conditions		

Abstract:
Many otherwise difficult challenges associated with drug delivery and biocompatible sensing, have become more tractable with the development of bottom up self-assembly techniques. DNA origami is a promising example of such. DNA origami are nanostructures composed of a long single stranded scaffold DNA strand, which is folded/stapled, in place by hundreds of synthetic oligomers, or staples. Extremely versatile, DNA origami can be folded into a variety of arbitrary 2D and 3D structures. Implementation of DNA origami in drug delivery, sensing, and potentially numerous future applications is hindered by a general lack of knowledge of their mechanical properties. This work seeks to develop a low-cost and accessible technique to measure DNA nanostructure mechanical properties by comparison. We compared four model DNA systems under shear conditions. The single stranded M-13 scaffold, and three origami folded from it. Namely, the 2D notched rectangle and 3D tetrahedron and tower. The relative robustness of the structures, compared to their scaffold, may be used to shed light on the impacts of folding on origami strength. This also opens opportunities for failure analysis via traditional imaging such as AFM/TEM.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Hengming Li		**Award Number**	70NANB18H050
Academic Institution: Appalachian State University		**Major:** Applied Physics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	I am planning to attend a graduate program that intersects the field of Neuroscience, Artificial Intelligence, Physics and Electrical Engineering.		
NIST Laboratory, Division, and Group:	Center of Nanoscale Technology (CNST), NanoFab Operation Group		
NIST Research Advisor:	Lei Chen		
Title of Talk:	Process Development for Area-Selective Atomic Layer Deposition using a Novel Photoresist		

Abstract:
Nanoscale film patterning is an essential part of the modern nanotechnology industry. As the sizes of nanodevices continue downward scaling, novel processing methods are needed to meet the increasingly difficult materials challenges associated with new devices. Typical fabrication of patterned structures requires multiple steps of deposition and etching which add complications and risks. Area selective atomic layer deposition (ALD) has shown promise for deposition of patterned structures with sub-nanometer thickness control, conformality, and uniformity of the deposited films due to its self-limiting growth process. However, it remains a challenge to selectively deposit a thin film on a desired patterned area. Here, we use a novel photoresist that exhibits good thermal stability and hydrophobic properties to minimize the thermal ALD thin film growth on its surface to selectively define the growth site.

The surface patterning begins with coating the fluorinated Orthogonal OSCoR AM1000 photoresist on a silicon wafer followed by exposure and development to obtain a patterned wafer. Different exposure dose and development time have been optimized to remove the residuals in the developed area. It was demonstrated that two consecutive 25 seconds development and a dose of 50 mJ/cm^2 yielded no resist residue in the developed region. The sample is then coated by Al_2O_3 using thermal ALD at varied temperatures. The results demonstrated that this new fluorinated OSCoR AM1000 photoresist can survive the high-temperature ALD process at 300C. The photoresist has potential to ameliorate the process complexities associated with nanofabrication. By exploring various ALD conditions and post-ALD processing, we are working towards our goal to improve the film contrast and the selectivity of ALD growth.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Thomas Marsh	**Award Number** 70NANB18H080
Academic Institution: Hamilton College	**Major:** Physics, Computer Science
Academic Standing (Sept. '18):	Junior
Future Plans (School/Career):	After graduating Hamilton College, I plan on attending graduate school to continue my studies of Physics
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Technology, Electron Physics Group
NIST Research Advisor:	Mark Stiles / Alice Mizrahi
Title of Talk:	Solving the Shortest Path Optimization Problem using a Memristive Network

Abstract:
Ant colony optimization is an efficient algorithm for solving the shortest path in a graph problem, inspired by how ant colonies find the shortest path to a food source without supervision. Currently, software implementations of ant colony optimization can solve numerous optimization problems, by mapping them to the shortest path in a graph problem, but their efficiency is limited by the high energy consumption of traditional computer chips. We propose a method to solve the shortest path problem using nanodevices called memristors. Memristors are resistors whose resistance depends on how much current has flowed through them in the past. A network of memristors can be made to represent any arbitrary graph. When voltage is applied across the network, the current will primarily flow along the shortest (i.e. less resistive) path through the circuit. This then causes the resistances of the memristors on the shortest path to decrease, creating a feedback mechanism that functions similarly to ant colony optimization. Previous works have proposed applying a constant voltage across the memristor network; however, we show that this method requires knowledge of the shortest path length. We propose a new method, which uses a voltage ramp, and does not require any knowledge about the graph. Through numerical simulations of randomly-generated graphs, both with Python and the circuit simulator Cadence, we show that our method successfully solves graphs with a wide range of sizes and topologies. We also show that the time and energy required to solve a graph scales with the shortest path length, whereas existing shortest path algorithms scale with the graph size. Due to the intrinsic parallelism of our approach, it has the potential to be faster and more energy-efficient than existing methods. Our results open the path for the implementation of hardware dedicated to optimization tasks.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Holland Rhodd-Lee	**Award Number** 70NANB18H073
Academic Institution: Wellesley College	**Major:** Neuroscience and Music
Academic Standing (Sept. '18):	Senior
Future Plans (School/Career):	Graduate Studies in Neuroscience
NIST Laboratory, Division, and Group:	Center for Nanoscale Science & Technology, 620.04, Nanoscale Imaging & Spectroscopy Group
NIST Research Advisor:	Mandy Esch, Darwin Reyes-Hernandez
Title of Talk:	A New Approach to Measuring Neuronal Differentiation in P19 Embryonal Carcinoma Stem Cells

Abstract:
Stem cell research is a rapidly evolving field that has provided insight into the operation of many biological systems because they can be studied in vitro, and have pluripotent abilities. This project focuses on the P19 embryonal carcinoma cell line (P19 cells), derived from mouse, and its ability to perform neuronal differentiation when exposed to minute concentrations of retinoic acid. The neuronal differentiation process takes on average 6-8 days to complete and can be detected through morphological changes, as well as with micro electrode arrays (MEA) which can measure the electrical signals produced by neuronal cells. The use of electro physiological changes, recorded by MEAs, and microscopy allows me to document the physiological change of the P19 cells from stem cells to neuronal cells. If successful, this method could become a conventional method used in the field of stem cell research .

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Emma Rogers		**Award Number**	70NANB18H061
Academic Institution: Tulane University		**Major:** Biomedical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Development of small-scale biomedical electronics for applications in adaptive and rehabilitative medicine, hopefully with DEKA research!		
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Technology in the Nanoscale Imaging and Spectroscopy Group		
NIST Research Advisor:	Dr. Mandy Esch		
Title of Talk:	The Role of Directional Shear Flow in the Inflammatory Response of Endothelial Cells		

Abstract:
Pursuing regulatory approval for potential new medicines is often a high risk and low return investment of both time and money. Multi-organ microdevices, specifically those of the gastrointestinal 10-organ system, may provide additional pre-clinical methods for drug development. Replicating in vivo conditions in body-on-a-chip devices requires modelling drug metabolism with a high degree of accuracy. Studies have shown that endothelial cell alignment under directional fluid flow influences metabolite transfer between tissues. However, researchers have not adequately compared the effects of endothelial cell culture under (1) unidirectional shear and (2) bidirectional shear on the proteomic expression of inflammation. Instances of bidirectional shear in vivo include reperfusion following cardiac ischemia as well as other instances of reoxygenation in the presence of abnormal tissues such as tumors. In such cases, reperfusion injury occurs due to both (1) mechanical stresses causing cell swelling and rupture upon restoration of blood flow as well as (2) chemical stresses due to the recirculation of reactive molecules generated in the hypoxic environment. Consequently, conventional methods of endothelial cell culture under conditions of bidirectional shear flow may result in proteomic expression more consistent with states of abnormal physiological stress. Here we developed a single microfluidic device that reliably replicates both unidirectional shear and bidirectional shear. We anticipate that human umbilical vein endothelial cells (HUVEC) cultured under these two conditions would display different levels of proteomic biomarkers of inflammation, namely the upregulation of interleukin-6 (IL-6) and interleukin-8 (IL-8). These findings may help to standardize the directional parameters of shear flow required for an accurate representation of in vivo conditions.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Stephen Tovcimak Jr.		**Award Number**	70NANB18H110
Academic Institution: Colleges of Nanoscale Science and Engineering at SUNY Polytechnic Institute		**Major:** Nanoscale Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Attending graduate school or pursuing a career in the semiconductor manufacturing industry		
NIST Laboratory, Division, and Group:	Center for Nanoscale Science and Engineering, 620, NanoFab Operations Group		
NIST Research Advisor:	Liya Yu		
Title of Talk:	Fabrication and Characterization of the Surface and Interfacial Effects on the Directed Self-Assembly of Block Copolymers (BCPs)		

Abstract:
In the current landscape of nanoscale manufacturing, one of the most essential processes is photolithography. As feature sizes continue to shrink in modern semiconductor devices, the current deep-UV and i-line processes are quickly running out of room. Block copolymers (BCPs) self-assemble into patterns with nanometer-scale features making them attractive templates for emerging nanolithography and nanomanufacturing techniques. Since thin film self-assembly is strongly influenced by surface energetics, both surface and interfacial effects become particularly dominate and are necessary to control for consistent process outcomes. The BCP patterning processes that the IC industry is interested in require the use of an electron-beam writer or extreme-UV tool to create sub-50 nm patterns, but the feasibility of these tools is limited by throughput and costs.

By introducing i-line lithography, which is a widely available, low cost lithography approach, to the BCP process, we also investigate the potential applications of i-line lithography directed self-assembly behaviors. We explored two paths to achieving nanoscale features which include topographical and chemical guiding patterns. The topographic method relies on reactive ion etching to alter physical confinement widths and depths while chemical patterning relies on the alteration of surface chemistry with different types of brush layers. Throughout each of these steps, characterization was performed by an analytical tool set including a goniometer, a contact profilometer and scanning electron microscope (SEM). From this it can be seen that the specific PS-b-PMMA we are using prefers a higher surface energy to bond and assemble. It appears that depending on the guide properties, we can see the BCP assemble into cylinders as well as parallel lamellas. The cause of these differences appears to be related to the frequency and presence of physical disturbances and chemical alterations.

CTL

Last Name	First Name	Lab
Fan	Steven	CTL
Gezahegn	Hiwot	CTL
Warner	Morgan	CTL
Luckabaugh	Zachary	CTL (SHIP)

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Steven Fan		**Award Number**	70NANB18H153
Academic Institution: University of Maryland College Park		**Major:** Computer Engineer	
Academic Standing (Sept. '18):	Sophomore @ University of Maryland College Park		
Future Plans (School/Career):	Obtain undergraduate degree and considering attending graduate school.		
NIST Laboratory, Division, and Group:	Communications Technology Laboratory, Wireless Networks Division		
NIST Research Advisor:	Richard Rouil		
Title of Talk:	Video Streaming Models		

Abstract:
Network simulation models should incorporate all phenomena that may impact network performance so that they will generate meaningful results. One of the most important issues is using simulated network traffic sources that match sources that exist in the real world. Most current video streaming traffic models are implemented using a Constant Bit Rate (CBR) that provides packets of a fixed size arriving at regular intervals. However, actual video streams very rarely display this constant behavior, with data rate, packet sizes, and inter-packet intervals varying depending on factors such as the mechanics of the codec, or video content. Our goal was to define a process that can be used to build realistic video streaming models based on actual applications. This process comprises several different model building approaches and the metrics that can be used to compare them. Using this process, we modeled and evaluated a set of video streams with different operational parameters, and we proposed extrapolations and generalizations of those models. We developed analytical models by using statistical tools such as curve fitting and time series predictions to process data taken from sample videos. We evaluated these models using several goodness-of-fit metrics, and those models that best matched the predictions were incorporated into a discrete-event simulator for comparison with real video streaming applications. The process that we developed and validated can be reused and extended to model diverse types of applications and behaviors. Additionally, we provided a proof of concept implementation of our process and the models it generated reflect the behavior of real-world video streaming applications significantly better than previous models do.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Hiwot Gezahegn		**Award Number**	70NANB18H119
Academic Institution: University of the District of Columbia		**Major:** Computer Science	
Academic Standing (Sept. '18):	Junior at University of the District of Columbia		
Future Plans (School/Career):	Going to Grad school while pursuing career		
dNIST Laboratory, Division, and Group:	Communication Technology Laboratory (CTL), Wireless Networks Division (WND)		
NIST Research Advisor:	Mr. Wesley Garey		
Title of Talk:	Analysis and Validation of Mission-Critical Push-To-Talk (MCPTT)		

Abstract:
Mission-Critical Push-To-Talk (MCPTT) is a service used by public safety for voice communications that offers high availability/reliability, low latency, support for both group and one-to-one calls, talker identification, device-to-device direct communications, emergency calling, and clear audio quality. The criticality of this service means that it is very important to verify that the operational procedures fulfill the requirements and expectations of public safety users. For this project our main task is to model the MCPTT operations through the various state machines that represent MCPTT behavior, and to use these models to analyze and validate the protocols standardized by the 3rd Generation Partnership Project (3GPP). We began the modeling process by using the 3GPP standard documents to obtain a detailed understanding of the various MCPTT protocols. With this understanding, we used the Process Meta Language (PROMELA) and the SPIN model checker to describe and verify the protocols in a systematic and automated way. At the end of this process we obtained a listing of various issues in the MCPTT protocols, such as live-locks, deadlocks, and assertion violations. During the length of the program, we produced an initial set of models to represent various state machines. We used the development and analyses of these models to identify several issues in the protocols. These results prompted us to do further detailed research on the originating causes for these issues, and, after consideration of the severity and possible consequences, we plan to submit proposed solutions to 3GPP to amend and correct the currently published standards.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Morgan Ayla Warner		**Award Number**	70NANB18H116
Academic Institution: Tennessee Technological University		**Major:** Computer Engineering	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Pursuing a career in Aerospace technology and innovation		
NIST Laboratory, Division, and Group:	Communications Technology Laboratory, Wireless Networks Division		
NIST Research Advisor:	Dr. David Griffith		
Title of Talk:	Stop Interrupting Me(ssages)		

Abstract:

Future handsets for public safety personnel will utilize technology similar to current smartphones, but they will also be able to communicate via a direct radio link with each other (Device-to-Device (D2D)), rather than sending messages to each other via a cell tower. This feature is useful when cell towers are out of reach or damaged. Public safety D2D-capable handsets that are out of cell coverage pick time slots and frequency bands (resources) randomly. If multiple handsets pick the same resource, their transmitted messages will collide and may not be recoverable by the receiving handset. For example, D2D-capable handsets use Sidelink Control Information (SCI) messages to advertise data transmissions and tell receiving devices how to receive the data. If a receiver cannot decode the SCI message, it will miss the data.

We modified an example script from the LTE Toolbox in MATLAB and used it to simulate the transmission of SCI messages. We included the effect of randomly distributing devices within a fixed area and applied a standardized channel fading model developed by the 3rd Generation Partnership Project (3GPP).

Our previous work assumed that all colliding SCIs were lost. However, our work shows that the receiver was often able to decode one out of several colliding SCIs, even at relatively low Signal to Interference Ratios (SIRs). The low-loss rates of the SCIs are due to the robust methods devices use to transmit the messages. We found that when we randomly placed devices, the chance that a colliding SCI message would be decoded was dependent on both the SIR and the number of colliding messages.

We are now generating a set of decoding probabilities that can be used in our theoretical models to account for the impact of SIR, and we will publish our results during Fiscal Year 2019.

Name: Zachary Luckabaugh (CTL SHIP student)

School: Poolesville High School (Montgomery County, Maryland)

Mentor: Wesley Garey

Title: A Graphical User Interface for Public Safety Communications Simulations

Abstract:

Mission-critical push-to-talk (MCPTT) over LTE is a service used by public safety for voice communications, that supports both group and one-to-one calls, talker identification, device-to-device (D2D) direct communications, and emergency calling. Currently there is no device that supports D2D which is required by MCPTT when the device is in off-network mode. This why the Wireless Networks Division (WND) has extended a graphical user interface (GUI) written in Python to demonstrate and allow users to interact with live simulations based on the D2D and MCPTT models they have developed and maintain using the discrete-event, network simulator, ns-3 to perform research that provides guidance and insight to public safety.

The main task of this project is to update and enhance the current GUI. This requires replacing the underlying MCPTT model with a newer version, redesigning the layout of the simulated applications to exploit all the features of the models, and creating a replay mechanism that can be used to easily capture, create, and repeat simulations that are run using the GUI.

The design of the new GUI has been started and each of the enhancements previously described have been addressed but there are still many limitations and issues that exist. This talk will cover in detail the enhancements that were made and ongoing problems that still need to be addressed.

EL

Last Name	First Name	Lab
Aboul-Enein	Omar	EL
Antia	Rushad	EL
Arnold	James	EL
Bergeson	Jennifer	EL
Bichnevicius	Michael	EL
Bones	Lela	EL
Brannon	William	EL
Brassel	Alexander	EL
Burns	Christian	EL
Calvo	Angelo	EL
Capraro	Marco	EL
Carangelo	Christopher	EL
Carlin	Katrina	EL
Collins	Ann	EL
de Oliveira	Samuel	EL
Dean	Pablo	EL
Eusman	Nickolas	EL
Fiola	Gregory	EL
Fisher	Ryan	EL
Furrh	Jacob	EL
Galfond	Brian	EL
Garner	Jonathan	EL
Hubbard	Joshua	EL
Kim	Timothy	EL
Kraus	Harrison	EL
Kreitman	Meir	EL
Lai	Trinny	EL
Lewis	Alexander	EL
Li	Simin	EL

Last Name	First Name	Lab
Littrell	Christopher	EL
Lopez Moralez	Alejandra	EL
Luu	Vanda	EL
McIntyre	Timothy	EL
Miranda	Angel	EL
Mnev	Peter	EL
Norwood	Frederick	EL
Pandey	Abhinav	EL
Saar	William	EL
Seamone	Andrew	EL
Segarra	Esteban	EL
Serrano Torres	Luis	EL
Sorra	Justin	EL
Sun	Xinran	EL
Tamayo Claro	Cesar	EL
Walsh	John	EL

SURF Student Colloquium

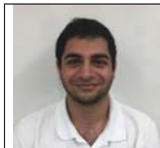
NIST – Gaithersburg, MD

August 7-9, 2018

Name: Omar Aboul-Enein		**Award Number**	70NANB18H103
Academic Institution: Salisbury University		**Major:** Computer Science and Mathematics	
Academic Standing (Sept. '18):	Graduate Student @ University of Maryland, College Park		
Future Plans (School/Career):	Starting this Fall, I am pursuing a Master's degree in Computer Science at the University of Maryland, College Park and intend to work part-time in the NIST Pathways program. Long-term, I hope to gain full employment at NIST as well as a PhD. in Computer Science to foster 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 a Manipulator-on-a-Cart		

Abstract:
Now in service and towards smart manufacturing assembly, a specific class of robots known as mobile manipulators offer more flexible and dynamic workflows within industry by freeing fixed manipulator arms from the limitation of operating on a single, calibrated workspace. The addition of a mobility component using a vehicular base allows a single robotic arm to perform assembly tasks at multiple locations. Further enhancing the flexibility is the concept of a manipulator-on-a-cart, whereby the robotic arm is now fixtured to a detachable cart that is moved and positioned by the base (i.e., transporter robot). A manipulator-on-cart unlocks further parallel workflows as a manipulator may now perform an assembly task while the vehicle independently services another payload on a cart. The payload may consist of static objects or another manipulator. The integration of a manipulator-on-a-cart requires careful calibration for proper utilization in today's manufacturing systems. Therefore, an acute understanding of the performance uncertainty and the problem posed by manipulator coordinate registration must be conveniently obtainable by users and manufacturers to ensure accessible and effective use of these manipulators. To foster this understanding within industry, the Robotic Systems for Smart Manufacturing (RSSM) Program has focused development on an accessible, cost effective, and artifact-based performance measurement concept. The uncertainty of the measurement concept was validated by comparing it to ground-truth defined by measurements taken with an optical tracking system (OTS).

The research conducted this summer focused on adapting and implementing the manipulator-on-a-cart scenario for testing with the artifact-based performance measurement method. Contributions included the development of remote communications between the manipulator and the newly acquired transporter robot, the design and implementation of concurrent robot control algorithms, and the evaluation of assembly-driven tasks utilizing the manipulator-on-a-cart. In addition, the implementation of the performance test method using the manipulator-on-a-cart was demonstrated at the ASTM Committee F45 meeting on Driverless Automatic Guided Industrial Vehicles held at NIST on July 31 – Aug 2, 2018.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Rushad Antia		**Award Number**	70NANB18H153
Academic Institution: University of Maryland College Park		**Major:** Computer Science	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Finishing school & finding a future in app/game development		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Network Control Systems		
NIST Research Advisor:	Richard Candell, Mohamed Hany		
Title of Talk:	localhost:3000/robotmonitor.html – Integrated Robot Monitoring System		

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 this, however, cannot sustain because of the high costs of installation and upkeep. This project's goal is to measure how reliable wireless communication (802.11b/g/n) works in a factory setting.

To do this, we plan on using two robot arms to work in a collaborative workspace. Then, parts of the robot workspace will be replaced with a wireless alternative. However, the problem lies in how to monitor these robots because each robot can have up to two extra pieces of proprietary hardware which makes it difficult to monitor all aspects of the robot. To do this we developed a monitoring system backend that allows for a single point of monitoring while hosting a front-end web interface. Along with a central logging system the front-end website can be useful for visualizing the robot data for demonstration purposes. Another feature is that the server can log all the data in .csv format for offline analysis.

The future work for the project will be to setup a communication channel for the two robots to interact on. This will be done by setting up each robot as a node in the Robot Operating System (ROS) and have them communicate through a master node. By using the ROS, the robots can communicate with each other to accomplish a collaborative task. After this is done we can see how a wireless environment can affect the performance of these collaborative robots.

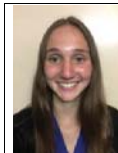
SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: James Arnold		**Award Number**	70NANB18H088
Academic Institution: Arizona State University		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Attend graduate school and pursue a career in robotics.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Engineering Laboratory Office, Smart Grid and Cyber-Physical Systems Program Office		
NIST Research Advisor:	Dr. Thomas Roth		
Title of Talk:	Creating a Database for Designing Energy Efficient Houses		

Abstract:
Improving the energy efficiency of homes can both reduce the unnecessary consumption of power and save homeowners money. The rise in the availability of internet-connected devices, such as smart home appliances, has made the integration of advanced power saving algorithms into homes a necessary step in reducing power consumption. However, many possible power saving algorithms exist, requiring that there be a way to store and then compare the results of the different algorithms. The goal of this project was to develop a method that allows for the creation and subsequent population of a database from live data. In order to simulate an environment to test different algorithms for cooling a house, a model house was equipped with a lamp, heat pump, and temperature sensor. Using LabVIEW, the lamp was controlled to mimic real weather conditions and the reaction of the house was monitored. Combining the weather data sent to the lamp, the temperature data collected in the house, and the algorithm used to control the house required designing an experiment that could exchange data between different types of simulations. The final program, written in Java, can be used to create a database that is populated by data collected from the house. One important goal of the project was to create a database that was not specific to the experiment with the model house, so that it is functional for any variation of the current experiment. Besides being general purpose, the database can be easily queried to perform data analysis and visualization. As more energy saving algorithms are produced and internet-connected home appliances are made available, this database implementation will allow researchers to collect and analyze their data, resulting in a cohesive understanding of what needs to be done to improve the energy efficiency of homes.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Jennifer Bergeson		**Award Number**	70NANB18H122
Academic Institution: Purdue University		**Major:** Aeronautical and Astronautical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Finish my undergraduate degree with a concentration in aerospace propulsion, then pursue graduate school and a career in astronautical propulsion.		
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:	Powering the Internet of Things: Harvesting Ambient Energy with Photovoltaics		

Abstract:
Ambient energy is a potential energy source for many low power devices, however, there is a lack of methods to harvest this energy. Proper energy harvesting methods could enable more remote deployments for devices in the internet of things, as well as reduce maintenance requirements. In this study, we explored the possibility of harvesting ambient light using photovoltaics. We used solar cells to charge a small battery through a custom circuit which allowed the solar cells to operate at their maximum efficiency. This circuit also had step-up voltage capability, for situations when the cells' output voltage was low. To test the circuit, we fabricated a dark enclosure which only allowed in the light of a variable intensity white light emitting diode (LED), and we used this set-up to do experiments under various light levels. We placed the cells in the enclosure, and measured the current and voltage going in and out of the connected circuit. In studying the custom circuit, we discovered an optimum input power around 1-1.6 mW where the efficiency of the circuit reached a maximum of 85-90 percent, an interesting finding that we had not previously seen. We also studied the power consumption of a wireless sensor network to see if the silicon cell and step-up circuit could charge a network node's battery. This study is leading towards a technology where the nodes of a sensor network could connect to one of the cell/circuit combinations to significantly extend node battery lifetime. Combining the circuit and solar cell with the network has applications for the internet of things because it eliminates the need to constantly perform battery replacement, and allows devices to function in a more "hands-off" way.

SURF Student Colloquium

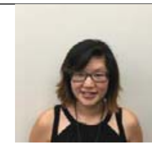
NIST – Gaithersburg, MD
August 7-9, 2018

Name: Michael Bichnevicius		**Award Number**	70NANB18H100
Academic Institution: The Pennsylvania State University		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Senior		
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:	Evaluation of a CO_2 Ground-Source Air Conditioner		

Abstract:
Heating, ventilation, and air conditioning (HVAC) equipment accounts for 40% of primary energy consumption in buildings. High-efficiency HVAC equipment is therefore necessary as part of the broader goal to develop net-zero energy consumption buildings. Ground-source (i.e. geothermal) heat pumps, as opposed to conventional air-source heat pumps, are a promising high-efficiency option for heating and cooling systems due to the stable, moderate temperatures in the ground.

This project studies the performance of a carbon dioxide (CO_2) ground-source air conditioner. CO_2 as a refrigerant has favorable environmental and thermophysical properties; however, it typically operates at very high pressures and in an inefficient transcritical cycle. CO_2 in a ground-source system, by contrast, may operate at lower pressures and in a more efficient subcritical cycle for much of the year.

A CO_2 ground-source air conditioner apparatus was evaluated in the laboratory under controlled conditions prescribed by ANSI/ASHRAE. The main factors which dictate performance include air and liquid flow rates, entering air dry bulb temperature and dew point, entering liquid temperature, and compressor frequency. Initial results show that the overall system performance based on air-side thermal capacity and electric power consumption is favorable. The results will be used as validation for a physics-based model of the CO_2 system. Future work includes testing a comparable geothermal system with R-410A instead of CO_2 as well as implementing both systems in the Net-Zero Energy Residential Test Facility (NZERTF) at NIST for further testing.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Lela Bones		**Award Number**	70NANB18H103
Academic Institution: Salisbury University		**Major:** Computer Science and Mathematics	
Academic Standing (Sept. '18):	Junior @ Salisbury University		
Future Plans (School/Career):	Attending graduate school with a research focus on brain computer interfacing (BCI)		
NIST Laboratory, Division, and Group:	Engineering Laboratory, System Integration, Information Modeling and Testing		
NIST Research Advisor:	Thurston Sexton		
Title of Talk:	Visualizing and Synthesizing Data from Maintenance Logs for Smart Manufacturing Analysis		

Abstract:

Smart Manufacturing aims to employ high levels of adaptability and computer systems integration to optimize the process of generating and producing goods. Industry has made a huge push in smart manufacturing research, however not every company has the budget or resources to make the transition to "smart." One of the areas where smart manufacturing is needed is in maintenance logs. Many come in the form of un-structured natural-language diagnostic databases filled with spelling and grammar errors. Nestor, a tagging application aims to help with this transition. Nestor is open source and works with the maintenance technicians to simplify and speed up analyzing and visualizing of maintenance databases. Due to the sensitive nature of the data, the process of transferring Nestor to industry application is difficult. There is an insufficient amount of public data to perform traditional analytics.

Nestor uses natural language processing (NLP) techniques to tag and structure very unorganized maintenance logs, My research goals are to build a visualization dashboard using the structured databases that comes from Nestor and to generate open source unorganized databases to test with Nestor and in the dashboard. Data is important, but is less useful without being able to properly visualize and understand the data. With my dashboard users will easily be able to load the document they generate through Nestor and receive a dashboard that easily visualizes their data. The dashboard is coded in Python and uses a library Flask to serve the web-based application. With the aid of Python libraries Bokeh and Holoviews, I create the visualizations that are displayed in the dashboard. Using Pytorch, a deep learning library native to Python, I create long-short term recurrent neural nets (LSTM) and train them on the data that is currently available to us. I then sample from the LSTM and create a character based language model that generates synthesized natural-language work orders.

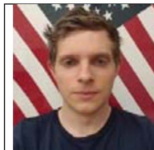
SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: William Brannon		**Award Number**	70NANB18H090
Academic Institution: Auburn University		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Graduate Student at Stanford University		
Future Plans (School/Career):	Pursuing a Ph.D. in Aeronautics and Astronautics with a research focus on advanced algorithms for the design of robust autonomous vehicles (i.e. Machine Learning, Motion Planning, Mapping, Localization)		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Inorganic Materials Group		
NIST Research Advisor:	LaKesha Perry		
Title of Talk:	Development of Automated Data Acquisition of Hydration Reactions in Microstructure		

Abstract:
The concrete industry uses several test methods to indirectly characterize the extent of reaction in cementitious binders. However, these methods do not access the actual reaction rates of the individual components as a function of the driving force, so there are significant gaps in our knowledge of reaction rates and mechanisms. This project is focused on automating the acquisition and analysis of reaction rate data for cementitious minerals using a continuously stirred batch reactor. LabVIEW™ programs are being written to control the instrument components and acquire data from a central location. Data will be analyzed using Python scripts for visualization and statistical modeling (e.g., regression). This project will therefore streamline the tasks of data collection, processing, and curation so that reaction rate information can be acquired routinely and used to build a cement reactivity data repository. These new capabilities will be demonstrated for the dissolution in water of gypsum, a mineral that is used routinely to regulate cement hydration and the major component of residential and commercial wallboard.



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August 7-9, 2018

Name: Alexander Brassel		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Computer Science, Mathematics, Operations Management and Business Analytics Triple Degree	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Attending graduate school		
NIST Laboratory, Division, and Group:	Engineering Lab, Systems Integration Division, Process Engineering Group		
NIST Research Advisor:	Dr. Boonserm Kulvatunyou		
Title of Talk:	Demystifying the performance bottleneck in Rich UI Web-based Applications		

Abstract:
Standardization of intercompany and interdivision communications is an important topic. To this end, Dr. Kulvantunyou and others have developed a full stack web application to allow companies to more effectively collaborate to develop and use standards for communication according to international standard methodologies. The web application is a rich UI with potentially intensive data transaction. Existing performance testing tools do not allow for pinpointing the performance bottleneck whether it is on the client or the server side; and they do not have an intuitive UI for non-developer users. This talk will describe an enhancement made to an existing opensource web application test tool to address these issues.

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August 7-9, 2018

Name: Angelo Calvo		**Award Number**	70NANB18H116
Academic Institution: Tennessee Technological University		**Major:** Manufacturing Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	After graduation, I plan on pursuing a career in industry before getting my masters in Engineering Management		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group		
NIST Research Advisor:	Dr. Guodong Shao		
Title of Talk:	Case studies for model based requirement generation using the VVUQ pattern		

Abstract:
Model requirements act as a vital foundation to any engineering model throughout the model lifecycle including model development, model deployment, model maintenance, and model end of life. Without this proper foundation, the goals of the model would not be completely identified and the technical stakeholder requirements, especially the model verification, validation and the uncertainty quantification (VVUQ) aspect, would not be correctly completed. As part of deliverables for the ASME model life cycle VVUQ interaction working group, a framework based on the model VVUQ pattern had been developed to make the generation of model requirements easier and more complete. The model VVUQ pattern can be applied to physics-based, data driven, or hybrid models.

In this project, a physics based model case and data driven model case are applied to the VVUQ pattern to demonstrate the generation of model requirement based on the framework. By applying the VVUQ pattern, the case studies identify the model stakeholder requirements and technical requirements for both a physics-based model and a data driven model. The case studies will not only help model developers and users determine the specific model requirement with VVUQ considerations, but also help standard developers distinguish what is necessary and unnecessary for developing the model requirements. Testing and verification of the VVUQ pattern will provide valuable feedback to the standard developers and in turn enable the improvement and enhancement of the ASME standard.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Marco Capraro		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Computer Engineer	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	After finishing my undergrad at the University of Maryland, I plan to attend graduate school and finish the remaining studies for my field		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Cognition and Collaboration Systems Group		
NIST Research Advisor:	Brian Weiss		
Title of Talk:	Data Management Strategy		

Abstract:

Manufacturing technology is evolving at a rapid pace with the emersion of advanced sensors, instrument-laden disruptive technologies including robotics and additive systems, cutting edge algorithms to filter and process disparate data streams, and novel user interfaces to enable human consumption of this new-found intelligence. These advanced capabilities have bred innovative monitoring, diagnostics, and prognostic technologies, especially those that can be integrated into manufacturing environments to enhance maintenance and control strategies to prolong process life through greater equipment awareness.

The National Institute of Standards and Technology (NIST) has a project focused on developing the necessary measurement science to design, deploy, verify, and validate these emerging monitoring, diagnostic, and prognostic technologies within manufacturing operations. The goal of this summer research effort is to develop and conduct the preliminary implementation of a data management strategy to capture data from a robot work cell that is serving as a NIST test bed. This data management strategy will afford NIST researchers with the capability of capturing diverse data streams (e.g. PLC process files, environmental videos) at specific, user-defined variables including resolution, frequency, and duration.

A comprehensive graphical user interface (GUI) will incorporate pre-defined capture plans and data collection parameters to enable users to obtain their most preferred data sets given their experimentation objectives and work cell operations. Individuals sets of data in the form of raw robot data, log files, and high-resolution recordings will be extracted from multiple devices within our lab through varying communication protocols and compiled onto one computer for ease of access. These devices include two environmentally-mounted video cameras and a PLC that will all be connected via the lab's internal network. This data will be captured and stored in a way that promotes efficient processing for diagnostic and prognostic analysis.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Christopher Robert Carangelo	**Award Number** 70NANB18H096
Academic Institution: Loyola University Maryland	**Major:** Mechanical and Materials Engineering
Academic Standing (Sept. '18):	Junior
Future Plans (School/Career):	Pursuing a Career in Aerospace Design
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Inorganic Materials Group
NIST Research Advisor:	Scott Jones
Title of Talk:	Development of Cement 3-D Printing Test Artifact

Abstract:
An artifact also known as a test print is a single object or series of objects or patterns that test the capabilities of a 3D printer such as accuracy, overhang tolerance, speed, etc. These artifacts are readily available for most fused deposition modeling printers (polymers), stereolithography printers (resins), and now some selective laser sintering printers (metals/ceramics/glasses). The problem we face is developing an artifact that can effectively test a paste printer that prints with a cement mixture. What makes these printers harder to deal with is the fact that cement does not set immediately set when printed with unlike resins, polymers, and metals. This leads to difficulty building objects with any high degree of accuracy or consistency. We first determined limitations that the printer had for structures, and details. We decided the best way to test the printer was using series of lines in different patterns which helped us look at several properties at once with each test. For example, we used a volume test that would determine nozzle offset, as well as volume tolerance by printing a series of lines varying in length. Through several of these tests determined how precise and fast the printer could run as well as the volume tolerance. We additionally found methods on how to improve these qualities by changing the code that runs the printer. In the future we hope to solidify these tests by developing highly detailed instructions that would allow anyone, scientists, hobbyists, engineers etc. to calibrate or test the effectiveness of their paste printer both on small and large scale.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Katrina Carlin	**Award Number** 70NANB18H037
Academic Institution: New College of Florida	**Major:** Chemistry
Academic Standing (Sept. '18):	Senior
Future Plans (School/Career):	Graduate from New College and work in the field before attending an analytical chemistry Ph.D. program
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group
NIST Research Advisor:	David Goodwin
Title of Talk:	Accelerated Weathering of Graphene-Polymer Nanocomposites

Abstract:
Graphene is an allotrope of carbon, composed of a single layer of sp^2-hybridized benzene rings, and is considered a nanomaterial due to its nanometer scale thickness. Graphene's structure provides it with great tensile strength, electrical conductivity, and thermal stability. Graphene can be incorporated into polymeric materials to provide these properties to the polymer system, and make the resulting polymer nanocomposite useful in a wide variety of products. Polymeric materials often degrade over time via natural processes, especially outdoors (i.e. heat, humidity, and UV radiation), thus it is important to investigate the effect of graphene nanofillers on the polymer degradation process. This study sought to investigate the implications of using graphene nanofillers in polymeric materials with respect to the service life of products, as well as the potential health and safety risks that may be associated with graphene-polymer nanocomposites. Two commonly used thermoplastics in products, low-density polyethylene and near polypropylene, were prepared with and without graphene via melt mix-extrusion to produce neat polymer controls and 1 % (by mass) graphene-polymer composites. The samples were placed in the SPHERE (Simulated Photodegradation via High Energy Radiant Emissions); the SPHERE is an accelerated weathering device that irradiates samples uniformly with UV light (140 W/m^2 at wavelengths from 295 nm to 400 nm). The SPHERE has individual chambers in which temperature and humidity can be controlled; the samples and controls were weathered at high temperature (55 °C) under dry (0 % RH) and high humidity conditions (75 % RH). The same conditions were replicated in chambers without UV light to understand the specific effects of temperature and humidity on the degradation process. The samples and controls were characterized before and after various timepoints of weathering via gravimetry, Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR), Raman Spectroscopy, and Scanning Electron Microscopy (SEM). Mechanical testing was also performed on samples and controls before and after weathering.

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August 7-9, 2018

Name: Ann Collins		**Award Number**	70NANB18H106
Academic Institution: Stevens Institute of Technology		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Serving in the U.S. Navy as a Nuclear Engineering Submarine Officer		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Applied Economics Office, Community Resilience Division		
NIST Research Advisor:	Jennifer Helgeson, Juan Fung		
Title of Talk:	Community Resilience		

Abstract:
Infrastructure within a community is a system of systems; if there is failure in one part, it is likely that the entire system will be disrupted. Currently, disaster-related loss (damage) estimates are available, but they tend to focus on direct loss only, are at aggregated levels, and provide lagged indicators. These estimates often fail to consider down-stream, indirect, and sustained effects, such as business interruption and loss of capacity on the establishment-level, which can be large and have a significant effect on the short- and long-term stability of a local or regional economy. For this reason, community resilience planning should take place ahead of time; vulnerable structures should be properly reinforced against potential hazard events and social and economic dimensions of the community need to be recognized. This project aims to advance research on the economics of community resilience generally, as well as the economics of seismic retrofit projects more specifically. Using three different locations at varying points of post natural disaster relief, San Francisco, Lumberton, and Puerto Rico, research was conducted on how best to prepare for these types of events. The research from San Francisco, CA is centered around calculating the financial burden to prepare for the next inevitable natural disaster. For Lumberton, NC, researchers are analyzing a formal survey data set to draw some conclusions from the outcomes of business interruption. Lastly, Puerto Rico is unique because it is an initial assessment to create a sample frame for a 2-3-year project under the NIST technical investigation of Hurricane Maria. Identifying these preventative actions will lay the ground work and result in important insights, leading to recommendations to improve recovery and resilience practices for communities facing risks from hurricanes, earthquakes, and other windstorms.

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August 7-9, 2018

Name: Samuel de Oliveira		**Award Number**	70NANB18H117
Academic Institution: University of Central Florida		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Recent graduate from UCF		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems (731), Polymeric Materials (04)		
NIST Research Advisor:	Dr. Andrew Fairbrother		
Title of Talk:	Degradation of Field-Exposed Photovoltaic Backsheets		

Abstract:
In a drive to bring solar energy into cost parity with other energy sources, manufacturers of photovoltaic (PV) modules are turning to newer, cheaper materials for certain module components. Some materials, such as non-fluoropolymer backsheets, are not always adequately field-tested. The backsheet is critical to the integrity of the module, providing electrical insulation and acting as a barrier to environmental stresses. Accelerated tests are designed to expose PV components to the main environmental stresses the module will endure during field exposure—however, accelerated test protocols sometimes fail to replicate real-world degradation mechanisms. The aim of this research is to understand the degradation of backsheet materials in field-exposed PV modules. 38 modules deployed for 0-28 years were retrieved from different climates for analysis. Color and gloss measurements, as well as FTIR-ATR and Raman spectroscopy provide qualitative and quantitative indications of backsheet degradation on the outer and inner layers. Trends for different climates and exposure times were identified. Additionally, localized differences in backsheet degradation at the cell and module level are found. Reasons for the inhomogeneous degradation of backsheets are discussed. The information collected from returning field-modules can be used to validate existing or create new accelerated testing protocols.

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August 7-9, 2018

Name: Pablo Dean		**Award Number**	70NANB18H153
Academic Institution: University of Maryland – College Park		**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Continue exploring the various fields of chemical engineering.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Inorganic Materials Group		
NIST Research Advisor:	Dr. Paul Stutzman		
Title of Talk:	Mineralogical Phase Analysis of Portland Cement by X-ray Diffraction and Scanning Electron Microscopy		

Abstract:

Portland cement is the most common hydraulic cement, used in a wide variety of construction applications. Once mixed with water, the cement's mineralogical components hydrate, crystallizing into an interlocking mass that provides the structural foundation of concrete. The cement minerals, referred to as "phases", serve a specific role in this hydration process as well as contribute to the resultant concrete's physicochemical properties, such as sulfate-resistance and amount of heat evolved during hydration. Hence, determining the mineralogical composition of Portland cement powders is critical to predicting how they perform. However, many methods today fall short in quantitatively and qualitatively characterizing cements.

With the use of X-ray powder diffraction (XRD) and scanning electron microscopy (SEM), one can not only determine the mass fraction of a certain mineralogical phase, but also its surface area. In this project, it was investigated how to most effectively use these two techniques, with a specific focus on enhancing the imaging process so as to account for the presence of all possible phases as well as quantify those phases' respective surface areas for the ultimate purpose of creating performance prediction models. The data collected will serve a critical role in developing models that can predict how a cement will perform based upon phase abundance, bulk chemistry, and texture, thus foregoing the need for long-running and expensive physical testing.

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August 7-9, 2018

Name: Nickolas Eusman		**Award Number**	70NANB18H065
Academic Institution: Worcester Polytechnic Institute (WPI)		**Major:** Mechanical Engineering and Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Finish my Bachelors in Science		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Networked Control Systems group		
NIST Research Advisor:	CheeYee Tang		
Title of Talk:	Railroad grade crossing simulator for use in cybersecurity testbed		

Abstract:

The uncovering of Stuxnet in 2005 was a wakeup call for many major security flaws within Industrial Control Systems (ICS). The control systems industry has always been outdated for several different reasons including: necessity for constant use, little time given to maintenance or software upgrades, and unwillingness for users to change what already works. This leaves many kinds of vulnerabilities within ICSs. To create standardized safety practices to protect the ICS industry, security measures that suit the unique requirements of each ICS must be implemented.

The project objective was to simulate a railroad grade crossing for use in a cybersecurity testbed. These systems are common across the US, where there are more than two hundred thousand railroad grade crossing signal systems. The grade crossing simulator created in this project consists of three major components. First, the train location sensor. Since we cannot have the real sensor in our lab, we use simulation to emulate its output. Second, the communication channel between the sensor and controller. We sample sensor voltage, convert it to digital signal, and communicate to the controller via the Controlled Area Network (CAN). Third, the Programable Logic Controller (PLC). The controller collects sensor data and, using the control algorithm, calculates the proper timing to activate safety mechanisms such as gates, buzzers and lights.

For this summer, the focus of the project was completion of the first two components described above. To accomplish this, the sensor data was created by converting a digital output from a Beaglebone Black to an analog signal using a resistor–capacitor (RC) circuit and pulse width modulation. The output voltage was received by an analog to digital to CAN converter. This device's CAN signal is received by a Beaglebone Blue, until hardware is acquired so the signal can be received by a commercial PLC. Once integrated with the PLC, this system can be used in the testbed.

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August 7-9, 2018

Name: Patrick Feeney		**Award Number**	70NANB18H130
Academic Institution: University of Rhode Island		**Major:** Computer Science & Mathematics	
Academic Standing (Sept. '18):	Senior at University of Rhode Island		
Future Plans (School/Career):	Graduate Studies in Computer Science		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Engineered Fire Safety Group		
NIST Research Advisor:	Kevin McGrattan		
Title of Talk:	Automated Translation of MATLAB Programs to Python to Increase Accessibility and Cross-Platform Compatibility of Open Source Software		

Abstract:
While MATLAB has been a common language for scientific computing in the past, the widespread adoption of Python in the last decade has challenged MATLAB's position as the dominant language in scientific computing. The fact that MATLAB is a proprietary language limits its usability in open source and cross-platform software. MATLAB programs require an expensive license to run, limiting the accessibility of the program for potential open source contributors. The fact that MATLAB is closed source results in issues with cross-platform support. Program developers are unable to resolve inconsistencies in program behavior between platforms since they are unable to change MATLAB's source code.

MATLAB is still widely used even though Python is both free and open source. The large amount of code written in MATLAB and the difficulty in adapting this code for a new language can deter developers from translating their programs. This has led to several attempts to develop software to translate MATLAB programs into Python programs. We have expanded on one such project, the "Small MATLAB and Octave to Python compiler" or SMOP by Victor Lei, to create a translator with design goals differing from older translator projects.

Older translator projects attempted to translate MATLAB programs into Python programs by utilizing large custom libraries emulating MATLAB's functionality. This caused the generated Python code to be extremely difficult to understand and further develop. This lead to the necessity of maintaining the original MATLAB programs instead of focusing on the development of the Python programs. Our version of the SMOP translator aims to emulate MATLAB's functionality using existing Python modules for scientific computing whenever possible. This allows for our generated Python code to be maintained after the MATLAB code that generated it has been deprecated. By creating such code, open source projects can benefit from the greater accessibility and cross-platform compatibility of Python.

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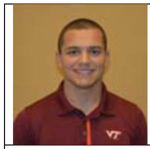
Name: Gregory Fiola		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Fire Protection Engineering	
Academic Standing (Sept. '18):	Graduate Student @UMD		
Future Plans (School/Career):	Continue Fire Research in graduate school		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, National Fire Research Laboratory		
NIST Research Advisor:	Dr. Rodney Bryant		
Title of Talk:	Calorimetry Reflexes: Characterizing Response Time of Fire Measurements		

Abstract:
The National Fire Research Laboratory (NFRL) houses an array of exhaust hoods that have the capability of accurately measuring heat release rate (HRR) from fire experiments using the principle of oxygen-consumption calorimetry. Heat release, specifically peak heat release, is an important parameter for evaluating the potential spread of hazardous conditions due to fire. In an effort to improve fire safety, it is important that the limitations and uncertainties of HRR measurements are considered, particularly with respect to system time response. Inherent to every measurement contributing to the HRR calculation is a response time that limits the system's ability to fully resolve transient fire events, such as ignition and flashover. Measurements of HRR are commonly reported solely as peak HRR and are heavily relied upon for characterization and classification of fires, yet peaks are resolved inconsistently from facility to facility as well as across experimental configurations. Several existing methodologies of characterizing response times are evaluated, including step function response, square wave response, and comparisons to mathematical models. An improved method is proposed, the 'waveform' methodology, consisting of a pulse train of repeating square waves. This waveform can be processed as a bi-level signal, unlocking well-established signal processing theory and tools (such as rise times and contrast functions) for better characterization of dynamic response. Waveform analysis has shown to be a robust method of resolving time response separate from transport delay, revealing an overall system response time of about 7 s. Results of this research are to improve fire metrology and understanding of limitations of calorimetry measurements, allowing for more accurate and informative reporting of HRR and flammability characterizations of products and materials.



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Name: Ryan Fisher		**Award Number**	70NANB18H109
Academic Institution: Virginia Polytechnic Institute and State University		**Major:** Aerospace Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing a career in aerospace engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Life-Cycle Engineering Group		
NIST Research Advisor:	Guodong Shao		
Title of Talk:	Testing of the MTConnect - OPC-UA Companion Specification		

Abstract:
Smart Manufacturing (SM) is the future of the manufacturing industry. Seamless, accurate, and fast connection and communications among devices are critical for SM. By leveraging information technologies, devices can dynamically communicate with each other to increase factory production, while decreasing engineering costs. Open Platform Communications - Unified Architecture (OPC-UA) facilitates such communication. The OPC-UA is a platform-independent standard through which various systems and devices can communicate by sending messages between clients and servers over various networks. OPC-UA enables syntactic interoperability between clients and servers. MTConnect is another a manufacturing interoperability standard that provides a semantic vocabulary for manufacturing equipment to provide structured contextualized data with no proprietary format. MTConnect data sources include production equipment and sensor packages, while its Extensible Markup Language (XML) data format provides both human and machine-readable features. Integrating the two standards will provides companies powerful interoperability capabilities. MTConnect OPC-UA Companion Specification has been developed to serve this purpose.

The goal of this project is to test the current version of the MTConnect OPC-UA Companion Specification. This specification sets a standard means of communication between MTConnect devices and OPC-UA Clients/Servers based on XML structures. To implement the standard, the following components must be created: an OPC-UA Server, an OPC-UA Client, a converter that translates data structures in MTConnect XML format to MTConnect OPC-UA Companion XML format that can be recognized by the server, simulated test case data in MTConnect XML format, and a MTConnect XML data parser. The activities of the standard testing include passing in varying data structures/objects through the server and confirming the information is received accurately by the client. The findings of the standard testing will be provided to the standard development organization for improving the future versions of the standard.

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Name: Jacob True Furrh		**Award Number**	70NANB18H125
Academic Institution: University of Houston		**Majors:** Environmental Sciences & Civil Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Graduate school in Environmental Engineering followed by applied science and engineering research		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Wildland-Urban Interface Group		
NIST Research Advisor:	Dr. Erica Kuligowski		
Title of Talk:	Hurricane Maria: Reconstructing Flood Hazards through Emergency Messaging		

Abstract:

On Sept. 20, 2017, Hurricane Maria made landfall along the east coast of Puerto Rico as the strongest hurricane to strike the island since 1928. The storm left a wake of devastation through intense winds, storm surge, rainfall flooding, and landslides. The National Construction Safety Team (NCST) Act authorizes NIST to investigate building performance, emergency response, and evacuation procedures in the wake of any building failure that has resulted in substantial loss of life or that posed the potential for substantial loss of life. An analysis of emergency communications prior to and during the storm is essential to diagnosing evacuation/sheltering procedures and implementing a survey to obtain much needed data on the experiences of evacuees and residents across the island. Textual analysis was performed on over 500 National Weather Service messages sent out in the 48 hours prior to and after landfall, many of which are flood-related. Datasets on flooded municipalities, individual townships, and rivers were extracted and imported to ArcMAP. The resulting maps, composed of multiple emergency messages and reports using 30-minute intervals, can be used as a decision support tool to choose adequate sampling locations for NIST's NCST technical investigation of Hurricane Maria and its impacts on Puerto Rico. This research is preliminary, as part of a multiyear investigation and will be used in combination with other resources.

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August 7-9, 2018

Name: Brian Galfond		**Award Number**	70NANB18H095
Academic Institution: Catholic University of America		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Production Systems Group		
NIST Research Advisor:	Gregory Vogl		
Title of Talk:	Measuring and Diagnosing Machine Tool Errors Using an Inertial Measurement Unit and Inductive Proximity Sensors		

Abstract:
Many part-making manufacturing operations depend on machine tools to move cutting tools and workpieces to their desired location. These machine tools use linear axis that degrade over time with usage. Degradation can cause linear and angular errors, reducing the precision of manufactured parts. If these errors become too great, machine tools can unexpectedly fail and require downtime to fix, putting a halt on production. Due to failures, lost production time, and repair costs, the manufacturing industry loses tens of billions of dollars yearly due to an inability to routinely track machine tool health *in situ*. Previous work has shown that machine tool errors can be measured using an internal measurement unit (IMU) made of gyroscopes and accelerometers. The purpose of this project is to develop a method of measuring and diagnosing the health of the ball bearings in the trucks used within a linear axis. For our system, we removed and degraded balls from one of the four trucks before reinserting the degraded balls. After each additional degradation, the linear axis was moved at varying speeds as we measured linear and rotational signals with an IMU. Simultaneously, we used four inductive proximity sensors to track the phase due to recirculation of a ball loop within each truck. After aligning the phases, we observed how the linear and rotational error motions changed based on which balls were in contact with the rail. Moving forward, we hope to develop a diagnostic process that will use the error motion data along with the phase tracking data to recognize when truck maintenance should be performed.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Jonathan Garner		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	I plan to pursue graduate studies in Electrical Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Cognition & Collaboration Systems Group		
NIST Research Advisor:	Dr. Helen Qiao, Ph. D.		
Title of Talk:	Advanced Sensing Development to Support Robot System Prognostics 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 considerable 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 and a smart target with light pipes are used to test the robot's accuracy. A smart target prototype was developed with the ability to display multiple unique colors. A target identification and tracking algorithm was developed in MATLAB (then converted to C code) to determine the location and then the center of the smart target. The algorithm uses color filters, image filters, and differences in light intensity between the target and the background to determine the location of the target and its center. A graphical user interface (GUI) was created in C++ to implement the camera's software development kit (SDK) to control the camera and to implement multiple features such as video capture, video playback, and the target tracking algorithm. The target identification and tracking algorithm was implemented in C++ using the Open Source Computer Vision Library (OpenCV) to increase efficiency when compared to MATLAB and to work with the GUI. As the 7-D system nears its final design, the target identification algorithms will be calibrated and modified to function with the final motorized smart target that is constantly rotate toward the cameras. In the future, the algorithms will be used to track the target in real time 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.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Joshua Douglas Hubbard		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans:	Ph.D. in Chemical Engineering		
NIST Laboratory, Division, and Group:	Engineering Lab, Materials and Structural Systems Division, Polymeric Materials Group		
NIST Research Advisor:	Dr. Jae Hyun Kim		
Title of Talk:	Essential Work of Fracture and Digital Image Correlation Analysis of Crack Propagation in PET after Accelerated Weathering		

Abstract:
The durability of polymeric materials under service conditions is a critical aspect to be addressed when evaluating their potential in a wide range of engineering applications from building materials to photovoltaic backsheets. The relatively high mechanical strength and thermal stability of certain polymers have motivated researchers to investigate these properties as functions of various service conditions that typically contribute to the degradation of materials used in these applications (e.g. humidity, temperature, UV exposure). The Essential Work of Fracture method (EWF) has been identified as a quantitative approach for fracture characterization of such polymers at relevant sample thicknesses. The current work focuses on the fracture process of two commonly studied polymers; polyethylene terephthalate and polyester. The specific essential work value obtained through EWF experiments and analysis is theoretically dependent only on the thickness of the specimen, and therefore can be useful as an evaluation criteria of material toughness independent of other geometry. To apply this method and obtain an accurate result, it is necessary to validate the assumption that the ligament zone is completely yielded prior to crack propagation. In this work we use Digital Image Correlation (DIC) technology to track how plastic deformation in the ligament zone and the corresponding specific essential work value changes as a function of varying UV exposure conditions maintained by the Simulated Photodegradation via High Energy Radiant Exposure (SPHERE) at NIST. Preliminary results demonstrate a decrease in the specific essential work value as exposure times increase from 0 to 200 hours under the experimental conditions: 40 C, 70% RH, and 100% UV. In addition, DIC analysis of the strain field surrounding the ligament revealed a smaller region of plastic deformation for aged specimens. These results indicate that accelerated aging of the polymers for long periods (>160 hours) can lead to embrittlement and a corresponding decrease in the material's resistance to fracture.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Timothy Kim		**Award Number**	70NANB18H153
Academic Institution: University of Maryland College Park		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue career in Mechanical Engineering with some sort of programming involved		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Smart Grid Program Office, 730.04		
NIST Research Advisor:	Cuong Nguyen, Avi Gopstein, DJ Anand		
Title of Talk:	Solar Microgrid Performance and Optimization		

Abstract:
The cost effectiveness of photovoltaic energy and the technology associated with power conversion has enabled consumers of electric power to use it to supplement their dependence on grid delivered electricity. As this technology is driven even further, photovoltaic sources are being used to power self-sustaining electrical networks called microgrids. Microgrids provide certain advantages over a centralized system such as operating in islanded mode -providing a flexible means to harness various forms of renewable energy. Islanded operation of microgrids also presents some technical challenges. One challenge that I addressed in my work is the need for a method to simultaneously optimize a wide variety of technologies that must work together to ensure the performance of distributed energy sources. My work modeled multiple components of a photovoltaic system and considered all the inputs, outputs, and constraining conditions in a parametric study to optimize all the performance variables of the system. My presentation will demonstrate how this was achieved using data collected from an IV Curve Tracer, micro-PMUs and MATLAB based power system simulations. A 3-phase solar inverter and a GE Multi-Functional Relay have also been modeled.

SURF Student Colloquium

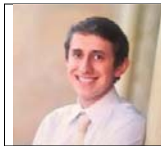
NIST – Gaithersburg, MD

August 7-9, 2018

Name: Harrison Kraus		**Award Number**	70NANB18H153
Academic Institution:	University of Maryland, College Park	**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a Master's of Science in Chemical Engineering at UMD		
NIST Laboratory, Division, and Group:	Engineering Lab, Material and Structural Systems Division, Structures Group		
NIST Research Advisor:	Marc Levitan		
Title of Talk:	Analysis of Garage Door Failures and Subsequent Effects on Residential Building Performance during the May 22, 2011 Tornado in Joplin, MO		

Abstract:
Of the various types of severe weather storms, tornados are considered one of the most difficult to study as their small area and high wind intensity makes it difficult to measure exact wind speeds. Tornado wind speeds are often estimated from the degrees of damage to damage indicators on the ground, though this is an imprecise method. The Enhanced-Fujita (EF)-5 tornado that hit Joplin, MO, on May 22, 2011, has presented the opportunity to improve these wind speed estimates with empirical data on tornado damage to one- and two-family residences. Data was collected using remote sensing imagery to determine the degree of damage to specific parts of the house (e.g. percent roof damage, exterior wall damage). And, wind speeds of this tornado were estimated independently of ground damage through a model using the pattern of tree fall over the area impacted by the tornado.

Garage door failure was explored as it has been seen in individual cases that garage failure can form a starting point for damage done to the other portions of the house. Probabilities of certain degrees of garage failure were calculated for varying ranges of wind speed in relation to factors such as garage size and orientation of the garage to the wind direction. Roof damage with respect to garage failure was also analyzed, as it has been hypothesized that garage door failure can lead to sudden increase in wind pressure inside the garage that can in turn damage the roof above the garage. Through this analysis, empirical data has confirmed that garage door failure can lead to increased wind damage to the rest of the house.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Meir Kreitman		**Award Number**	70NANB18H153
Academic Institution:	University of Maryland, College park	**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a career in product development		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Production Systems Group (735.15)		
NIST Research Advisor:	Jordan Weaver		
Title of Talk:	Characterization of Single Scan Laser Tracks on Nickel Super Alloy 625 Using Nanoindentation		

Abstract:
Additive manufacturing (AM) is a layer-by-layer process of building components using different materials and methods. AM can create parts that are impossible to make through other processes; however, AM is not the most established and reliable method for manufacturing. Some of the barriers to the wide spread adoption of AM include process variability, fabrication speed, part accuracy, and material properties. The latter is the focus of the current study that uses single scan laser tracks on a metal plate as a stepping stone to understanding laser based AM of metals. NIST has made thermographic, melt pool geometry, and microstructure measurements of single scan laser track experiments on nickel super alloy 625; however, mechanical property measurements of the laser track are lacking due to the difficulty of mechanically characterizing the small volume of material. Nanoindentation, which is the process of probing micron sized volumes of material, was used to address this gap to determine the modulus and hardness across the melted zone into the base material on laser track cross-sections. The results show the hardness changes from ~5.5 GPa in the melted zone near the surface to ~4.8 GPa in the base material for a laser track setting of 195 W and 800 mm/s. In comparison, the hardness shows no significant difference in the melted zone compared to the base material for a laser track setting of 195 W and 200 mm/s. The influence of crystal orientation, residual stress, and the dendritic microstructure that forms in the melted zone on the hardness response will be discussed. The use of nanoindentation to characterize single scan laser tracks can provide additional insight into the AM process and data for material models which will enable better predictions and optimization of additive material properties.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Trinny Lai		**Award Number**	70NANB18H102
Academic Institution: Regis University		**Major:** Chemistry and Mathematics	
Academic Standing (Sept. '18):	Graduate Student at Colorado School of Mines		
Future Plans (School/Career):	Attending Colorado School of Mines		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group		
NIST Research Advisor:	Stephanie Watson		
Title of Talk:	Analysis of Automotive Paints under Weathering Conditions		

Abstract:
Trace evidence is the remaining evidence that is transferred between people and objects after a crime. Paint chips, fragments, and smears are examples of trace evidence that can be used to solve many forensic cases specifically involving automobiles. For instance, in many hit-and-run accidents, small pieces of automotive paint are left at the crime scene. Those paint samples are then used to identify the cars of the suspects. However, the examinations of these paint samples only involve visual inspection which can be varied due to many external factors, such as different examiners and environmental conditions. Thus, the overall goal of this project is to find a better, relatively fast, and more quantitative method to analyze the paint samples in order to ultimately determine the car's make, model, and year.

One consideration in the analysis of automotive paints is its degradation, focusing on the outer layer or the clear coat. Since the clear coat is a polymeric material, weathering conditions such as ultraviolet (UV) radiation, heat and moisture can change the chemistry and lead to degradation. For this study, several clear coat paint samples were obtained from two manufacturers: BASF and PPG. Samples consisted of the clear coat applied on top of black and white base coat to determine the effect of color to the degradation process. All the samples were then exposed to weathering conditions using NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure). NIST SPHERE is an accelerated weathering device that independently controls temperature and humidity, and uniformly irradiates samples with high intensity UV light (140-165 W/m^2 at wavelengths from 295 nm to 400 nm). Samples were weathered approximately 2500 hours under extreme conditions: 55 °C ± 3.5 °C, 75 % ± 5 % relative humidity, and 100 % UV radiation. The instruments used in this study included attenuated total reflection- Fourier transform infrared spectroscopy (ATR-FTIR), colorimeter and glossmeter. Instrumental results were then examined for changes in chemistry as a function of weathering exposure.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Alexander Lewis		**Award Number**	70NANB18H094
Academic Institution: Trine University		**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a PhD in Electrical Engineering		
NIST Laboratory, Division, and Group:	Engineering Lab, Systems Integration Division 734		
NIST Research Advisor:	Boonserm Kulvatunyou, Nenad Ivezic		
Title of Talk:	Ontology Engineering for Interoperable Manufacturing Process Information		

Abstract:
To stay ahead of the competition, companies in the manufacturing industry must be as efficient as possible and minimize the time it takes to get products to market. Some inefficiencies that may hinder this include problems with interoperability in process and production planning, the lack of a common language between all departments involved in a manufacturing process, and the lack of an open system that allows for relevant data to be accessible to those who may require this information. The proposed way of overcoming these issues is using Process Specification Language (PSL) ontology. An ontology is a formal representation of a set of concepts within a domain and the relationships between those concepts. PSL is an ontology created by NIST for the manufacturing industry to represent process plans.

PSL was created for use in discrete manufacturing. The research question is whether it is possible to use PSL for all manufacturing processes, including batch and continuous manufacturing or is it necessary to improve PSL to allow for this. An experimentation package is needed to make this assessment. This package is to include instructions, ontology files, query files, and the software necessary to assess the power of PSL ontology in representing discrete, continuous, or batch process plans. Research is being done to relate PSL with batch and continuous manufacturing. Examples, explanations, and definitional instructions are being created to aid in the experimentation package.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Simin Li		**Award Number**	70NANB18H153
Academic Institution:	University of Maryland – College Park	**Major:** Mechanical Engineering & Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Complete Mechanical Engineering undergraduate and graduate degrees in preparation for a career in increasing productivity through engineering		
NIST Laboratory, Division, and Group:	Engineering Lab, Systems Integration Division, Group 12		
NIST Research Advisor:	Dr. Yan Lu		
Title of Talk:	Additive Manufacturing (AM) Bench Data Understanding and Processing		

Abstract:

Additive manufacturing (AM) is a highly attractive fabrication method because of its ability to produce complex parts that cannot be machined using tradition manufacturing techniques. However, inconsistency across AM parts in both performance and geometry is a large roadblock preventing wider adoption across industry. NIST has made significant strides towards improving traceability and repeatability in Additive Manufacturing, through a common AM data management system - the Additive Manufacturing Materials Database (AMMD), which captures data generated from the lifecycle of a AM part, from the builds to tests. In order to curate and share the information gathered from the NIST Additive Manufacturing Benchmark Test Series (AM-Bench), which were designed to challenge research organizations to create AM predictive models for LPBF based metal parts and material extrusion polymer parts., a modified AMMD data schema was developed in the summer and is presented here. From the AM-Bench challenges 01 and 02, the test series for LPBF processes, the importance and quantity of in-situ and post inspection data generated from the builds were investigated and recorded, noting assumptions and accuracy of tests and measurements. Combined with feedback from AM Bench modelers, the data schema was expanded to more fully capture process and testing parameters and the process-structure-property relationships. Overall, the modified AMMD data schema allows for a more comprehensive resource for researchers and institutions to share and query AM information.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Xiang Li		**Award Number**	70NANB18H092
Academic Institution:	George Mason University	**Major:** Computer Science	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Start Accelerated Master's program in Computer Science at George Mason University this fall		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Manipulation and Mobility Systems Group		
NIST Research Advisor:	Jeremy Marvel		
Title of Talk:	Predictive modeling of collaborative robot interactions		

Abstract:

In effective interaction between human and robots in manufacturing applications, safety and team efficiency are essential. One of the challenges is mutual understanding of the collaborative process between the robot and a human. To work effectively in the same work space, not only does each need to know the common goal of the task, but also to have a shared situational awareness of the environment and the process when proceeding to the final goal. Although the robot may shut down or sound an alarm when something goes wrong during an assembly task, humans do not necessarily realize when they are making a mistake. Therefore, it is important for the robot to understand the intent of the human and make decisions based on the information it receives from the human to reduce potential risks that may occur.

For this project, a set of labeled human image data was collected for training and testing purposes. This data set provides examples of a person either paying attention or not. The labeled images are then fed into a pre-trained object detection model from an open source framework application programming interface (API). This model uses a convolutional neural network to extract the features of the images and perform classification of the person's attentiveness.

As a result, the trained model can recognize and localize a person. It provides a level of confidence percentage with mapped labels to indicate whether the person is paying attention. The output information of the trained model will be used in further research, to help a robot to recognize whether the person with whom it is working is paying attention. This recognition is critical for the robot to determine its next action and to maintain a safe working environment.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Christopher Littrell		**Award Number**	70NANB18H091
Academic Institution: Carnegie Mellon University		**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Work in industry before pursuing graduate study in chemical engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group		
NIST Research Advisor:	Xiaohong Gu		
Title of Talk:	Analysis of the Degradation of Polymeric Components Used in Photovoltaic (PV) Systems		

Abstract:
One of the most important features when considering installing solar panels in the reliability of the solar modules inside. The long-term durability of these modules is dependent upon the proper function of multi-layer polymer backsheets, which act as electrical insulators and weathering protectors. However, environmental factors such as ultraviolet (UV) light exposure, heat, and humidity promote the degradation of these backsheets. Degraded backsheets leave the module open for molecules such as water vapor and oxygen to enter, which can hasten the delamination and corrosion of the solar cell inside. To test the service life of these backsheets, both an accelerated laboratory exposure method and an outdoor exposure method have been set up. The data collected will be important in investigating the correlation between the two types of exposure, with the aim of improving the accuracy of service life predictions of solar modules.

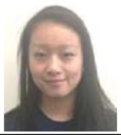
In this project, the accelerated laboratory exposure was conducted using either the NIST simulated weathering device, SPHERE, or a commercial xenon lamp device, in which samples were exposed to variable UV intensities under elevated temperatures and relative humidities. The outdoor weathering was carried out in the climates of Maryland, Florida, and Arizona. After receiving samples after designated exposure times, the extent of degradation was measured with changes in their optical, chemical, and mechanical properties in mind. Colorimetry and gloss were utilized in analyzing the optical signs that the backsheets had degraded. Attenuated total reflection - Fourier transform infrared spectroscopy (ATR-FTIR) was used in analyzing the changes in chemical spectra of the backsheet materials to determine the extent of degradation. Tensile tests were used to analyze the mechanical properties, such as yield strength and modulus, to assess the extent of the mechanical degradation of the backsheets. Finally, a novel test being developed at NIST that involves using microscopy and tensile tests simultaneously to analyze the propensity of cracking in the backsheets was also utilized to compare the different backsheet materials after UV exposure.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Alejandra M. López Morales		**Award Number**	70NANB18H128
Academic Institution: SUAGM – Universidad del Turabo		**Major:** Civil Engineering	
Academic Standing (Sept. '18):	Graduated (June 2018)		
Future Plans (School/Career):	Gain some experience in engineering firm. Take FE and PE exams, to become a licensed engineer. In time, pursue PhD in structural engineering.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division (731), Structures Group		
NIST Research Advisor:	Joseph Main		
Title of Talk:	Data Collection and Management for Critical Buildings to Support the Investigation of Hurricane Maria's Effect on Puerto Rico		

Abstract:
On September 20, 2017, Hurricane Maria made landfall in the US territory of Puerto Rico as a Category 4 storm with peak wind gusts of 155 mph. The hurricane caused extensive rainfall of up to 38 inches, coastal inundation levels as high as 9 feet and hundreds of landslides. The combined effects of these hazards led to 100% loss of power and running water, 95% loss of mobile communications and approximately $90 billion in economic losses, making Hurricane Maria the third costliest hurricane in the history of the United States. On February 2018, the NIST Director established a National Construction Safety Team (NCST) to conduct a technical investigation of the effects of Hurricane Maria on Puerto Rico. A key objective of the investigation is to characterize the performance of critical buildings, specifically hospitals and storm shelters, and to evaluate the adequacy of existing design standards and codes for these facilities, including selection criteria for storm shelters. The goal of this summer research project is to support the selection of critical buildings for detailed study as part of the NCST investigation. As part of this effort, comprehensive lists were compiled of hospitals and storm shelters in Puerto Rico, along with their geographic coordinates and other relevant information. Using the Google Earth Pro software, the critical buildings were organized by type, emergency management zone and municipality, allowing for easy selection and display of building locations along with aerial imagery from before and after the storm. Reports of damage to critical buildings are being gathered from different sources, and characteristics of the buildings and their surroundings are being evaluated from aerial images. This information will aid in selecting samples of representative buildings for detailed study as part of the NCST investigation, including wind tunnel testing to evaluate wind loads on selected buildings.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Vanda Luu		**Award Number**	70NANB18H101
Academic Institution:	University of Maryland, Baltimore County	**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	I plan to pursue a MBA or a Master's degree in Engineering Management after my bachelor's degree.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group		
NIST Research Advisor:	Dr. Li-Piin Sung		
Title of Talk:	Key Parameters Effecting Polyester Weathering		

Abstract:
Plastic is cheap and used in abundance in everyday items, but *how long will it last?* Over the last few decades, people have developed a dependency on plastics and these plastics must be durable. Unfortunately, these plastics will degrade until it becomes brittle and "fails", but *when will it fail?* Weathering exposure tests performed on polymers can determine when they "fail". Outdoor weathering exposure tests are unpredictable and can take months and years. On the other hand, laboratory accelerated weathering can produce degradation results in days. Another question arises, *can we use accelerated weathering outcomes to predict outdoor weathering and service life of polymer materials?* Currently at NIST, this question is being addressed with the established service life prediction research program using the Simulated Photodegradation via High-Energy Radiation Exposure (SPHERE) on different polymer materials. The polymers used in this program include polyethylene (PE), polyethylene terephthalate (PET), and polyethylene terephthalate glycol-modified (pESTER). The results from the PE system demonstrated accelerated weathering can be used to predict outdoor weathering. This program is being continued with PET and pESTER systems.

This study concentrates on the service life of pESTER. pESTER samples were exposed at different time intervals in the NIST SPHERE at different temperatures and UV intensities. The samples were removed for mechanical and chemical measurements to assess the degradation progress. Tensile testing measures the elongation at break, toughness, yield strength, and modulus of elasticity. Attenuated Total Reflectance-Fourier-transform Infrared Spectroscopy (ATR-FTIR) measures the chemical changes. The results from the SPHERE exposure are compared to the outdoor exposure and 0% UV exposure.

The initial results showed unexposed pESTER is more ductile than unexposed PET even though they are very similar polymers in terms of chemical structures. However, pESTER degrades and yellows faster than PET. According to the measurement data, UV light dominates the degradation of pESTER compared to 0% UV. We will continue this study with the effects of temperature and humidity on pESTER.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Timothy McIntyre		**Award Number**	70NANB18H153
Academic Institution:	University of Maryland College Park	**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Finish Bachelor's Degree and pursue graduate school		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Structures Group		
NIST Research Advisor:	Marc Levitan		
Title of Talk:	Analysis of Damage Parameters and Degree of Damage Variability in Residential Building Performance from the 2011 Joplin Tornado		

Abstract:
The overall goal of this project is to evaluate residential building performance during tornadoes to better understand their resilience to extreme winds and characterize tornado damage as a function of wind speed. Utilizing remote sensing data and satellite imagery from the 2011 Joplin Tornado that damaged over 7,000 homes, as well as public records for each residence, it is possible to determine information about these residences such as when they were built, construction material, roof pitch, presence of garages, porches, and other significant architectural features. Then, in accordance with the Enhanced Fujita (EF) scale damage indicator for one-and-two-family residences, the damage inflicted to various common features of residences is assessed. These results are compared to a wind field model developed in NIST's technical investigation of the Joplin tornado developed using tree fall patterns. This wind field provides estimates of the maximum windspeed and associated wind direction independent of structural damage. The results from analyzing each residence can be compared to this windspeed to find what visible degree of damage most accurately represents wind speed. This research will provide valuable information about variability in structural performance and the accuracy of the EF scale.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Angel G. Miranda | **Award Number** 70NANB18H128
Academic Institution: Universidad del Turabo | **Major:** Industrial and Management Engineering

Academic Standing (Sept. '18):	Senior
Future Plans (School/Career):	Graduate school for Operations Research
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials & Structural Systems Division, Community Resilience Group
NIST Research Advisor:	Ken Harrison
Title of Talk:	Infrastructure Support of Critical Buildings

Abstract:
With the increasing frequency of costly natural disasters around the globe there is a strong need to develop and improve critical infrastructure to be resilient to catastrophic events. These extreme weather events, such as Hurricane Maria, can leave crucial services nonoperational leading to millions of lives at risk. The National Institute of Standards and Technology (NIST) has initiated a large study of the numerous impacts of Hurricane Maria on Puerto Rico. This work focuses on one important aspect of the study, that of infrastructure support of critical buildings. Supporting infrastructure includes the energy, water and sewer, transportation, and wireless communication networks. NIST will be analyzing how infrastructure was impacted by the failure of these systems and ultimately making recommendations for their improvement.

Through proper infrastructure and network planning these systems can be strengthened. This research consists of two parts, mapping and reconnaissance, and model building. Infrastructure maps were assembled for use in Geographic Information System (GIS) mapping software. For example, wireless communications towers in Puerto Rico were mapped and geolocated with images of post hurricane damage.

Next, prototype computer-based models were constructed to further study infrastructure support of buildings and planning to increase resilience to disasters. Specifically, optimization models were formulated that seek to make improvements to infrastructure networks so as to maximize the distribution of essential goods during natural disasters of varying severity. Links, such as roads in a transportation networks, are typically built to withstand specific loads. These links must endure significant stress during natural disaster and many of them become unfunctional. By determining the optimal assignment of load resistance, on links, disaster relief efforts can be improved. The construction of a linear program allows for the efficient identification of solutions. Experimental results will demonstrate the potential applying modeling to maximize resource distribution during natural disasters.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Peter Mnev | **Award Number** 70NANB18H153
Academic Institution: University of Maryland College Park | **Major:** Mechanical Engineering and Computer Science

Academic Standing (Sept. '18):	Sophomore
Future Plans (School/Career):	Attend graduate school for a Master's degree in robotics and then pursue a career in robotics.
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Cognition and Collaboration Systems Group
NIST Research Advisor:	Craig Schlenoff
Title of Talk:	Analyzing Agility of Robot Systems through Simulation

Robot systems are implemented in a wide variety of manufacturing settings, enabling mass production by efficiently and quickly performing repetitive tasks. Unfortunately, it is still very difficult to repurpose a robot quickly and cost-effectively, a characteristic known as "agility". Additionally, robots cannot recover from errors they encounter during operation, outside of those that are easy to pre-define. Also, robots from different manufacturers are difficult to integrate into the same system due to a lack of a shared language. These problems make robot systems very rigid and unappealing to small-medium manufacturers.

Agility of robot systems is not only limited, it is also difficult to assess. The Quantitative Positional Task Level Success metric proposed by NIST could be used to do this. This metric assesses how well a robot system can perform a kitting task where one or more robot performs pick-and-place operations. The metric includes time to complete, distance objects moved, kitting process completion and number of failures. However, some of these would be hard to evaluate in a real-world environment due to the amount of positional data that needs to be gathered. Using a computer simulation that accurately represents physical effects such as friction is a good way to easily gather this information, though there are several hurdles that need to be addressed prior to using it.

The work I performed this summer aimed to improve the accuracy of the Gazebo physics-based computer simulator. The Agility Performance of Robotics Systems lab has two robots, both of which have their own kitting gripper. I added them to the existing Unified Robot Description Format models of the robots, and imported them into the Gazebo simulation. Furthermore, I explored options for making physics-based grasping work by adjusting various simulation parameters like damping and friction. Once an accurate simulation is achieved, it will be possible to apply various control algorithms and easily gather a lot of data to assess their agility.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Frederick Norwood		**Award Number**	70NANB18H114
Academic Institution:	University of Colorado Boulder	**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a career in electrical engineering, specifically robotics or photovoltaics		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Manipulation and Mobility Systems Group		
NIST Research Advisor:	Nicholas Dagalakis		
Title of Talk:	Measurement and Tuning of Motorized-Dynamic Bending and Calibration Machine to Test Disposable Human-Collaboration-Robotics Safety Artifacts		

Abstract:
The movement of manufacturing to countries featuring labor with low hourly wages over the last fifteen years has motivated the development of a new generation of industrial robots that can work side-by-side with human workers. This has created a new technology of Human-Collaboration-Robotics, which combines the intelligence and dexterity of humans with the strength, repeatability and endurance of industrial robots. Since most robots are powerful programmable moving machines, the safety of workers working around these robots has become a top priority for safety standards development that will provide guidance for a comprehensive risk assessment of the robot arm, its tools, its controller, and the whole operating workspace where humans might be present.

Several robot safety standards set limits on the movement speed of robots in the presence of humans to allow workers to escape and to minimize the impact force in case of an emergency. Although the impact force depends on several factors, one of the most important is the robot's momentum. A simple and inexpensive instrument called the Motorized-Dynamic Bending and Calibration Machine (M-DyBeCaM) was built to simulate impacts for various impact momenta and impact speeds.

To simulate the impacts more accurately and safely, the M-DyBeCaM instrument was calibrated using a laser interferometer and an impact stop switch was installed. Several proportional–integral–derivative (PID) controller gains were found to deliver a variety of impact speeds, however the motor powering the M-DyBeCaM was unable to achieve the fastest of the desired speeds. This work will improve the testing of human bio-simulant bone artifacts and allow greater understanding of human-robot collisions, leading to better safety standards for human-robot interaction.

SURF Student Colloquium

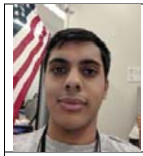
NIST – Gaithersburg, MD

August 7-9, 2018

Name: Abhinav Pandey		**Award Number**	70NANB18H153
Academic Institution:	University of Maryland, College Park	**Major:** Computer Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing a career in Computer Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Smart Grid and Cyber-Physical Systems Program Office		
NIST Research Advisor:	Eugene Song, Martin Burns		
Title of Talk:	A digital-twin of an IEEE 1451 smart temperature sensor for CPS/IoT research		

Abstract:

Cyber-Physical Systems (CPS) are integrations of physical and cyber components connected in a network that use computation to monitor and control the physical world using feedback loops of sensing and actuation. This project utilizes the Universal CPS Environment for Federation (UCEF), a toolkit to build co-simulations, and, the Institute of Electrical and Electronics Engineers (IEEE) 1451 standard, a network interface standard for smart sensors. IEEE 1451 network interface allows applications to remotely communicate with the sensors, such as, reading sensor data, as well as reading its Transducer Electronic Data Sheets (TEDS). The purpose of this project is to simulate a IEEE 1451 based smart temperature sensor in Java code effectively making it a "digital twin" of the real sensor. Different faults can be injected in this "digital twin" and its behavior and the responses it sends back can be analyzed to model how the sensor reacts to it including if it causes the simulated sensor to fail. These faults include setting the operating temperature outside the sensor's rated limit, setting the sensor's input voltage outside the rated limit, and disconnecting the sensor from the network. The long-term goal is to have hundreds of these sensors running in a co-simulation and analyzing what the side effects of one malfunctioning unit will have on the rest of the sensors and what will be some of the ways of minimizing these side effects. These results could then be used to integrate these smart sensors effectively in Cyber-Physical Systems and the Internet of Things.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Michael Roa		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Computer Science	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing graduates' degree in Robotics		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group		
NIST Research Advisor:	Moneer Helu		
Title of Talk:	Linking As-Planned and As-Executed Manufacturing Data in Near-Real Time		

Abstract:
The operation and maintenance of computer numerical control (CNC) machines can be improved by identifying discrepancies between the planned and executed manufacturing process. An approach suggested in the literature to identify such discrepancies is Dynamic Time Warping (DTW), which merges two datasets with disparate timestamps. However, current DTW methods require relatively large datasets, which limits its use for near-real-time monitoring. This research extends current DTW approaches using Windowed Time Warping (WTW), which can decrease the size of dataset needed for analysis. We implement WTW in a Java-based tool to improve the portability, computational speed, and accuracy of the analysis. Preliminary testing shows that WTW provides a near 115% faster compared to the current DTW approach. Such improvement highlights the value that WTW can provide for monitoring and optimization of smart manufacturing systems.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: William Saar		**Award Number**	70NANB18H153
Academic Institution: University of Maryland		**Major:** Fire Protection Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Master's Degree in Fire Protection Engineering from University of Maryland College Park		
NIST Laboratory, Division, and Group:	Engineering Lab, Fire Research Division, Wildland Urban Interface Group		
NIST Research Advisor:	Rik Johnsson		
Title of Talk:	Single and Double Fence Flame Spread in the Wildland Urban Interface		

Abstract:
The Wildland Urban Interface (WUI) is the zone of intersection between forested and developed areas. Structures and communities in this zone are at an increased risk of large-scale fire events, and are costly to protect (at an estimated annual federal cost of $3B). Firebrands (embers) have been identified as a significant mechanism of fire spread in WUI communities. Combustible structures such as fences, woodpiles, and decks, and combustible ground cover such as mulch generate firebrands when ignited that can be lofted and carried long distances by high winds to other ignitable fuel sources. Fences are efficient vehicles for flame spread as they allow for both firebrand generation and relatively fast lateral flame spread, especially when in a parallel two-fence configuration.

Experiments were conducted to determine the effect of fence type, fence material, ground cover, wind speed, parallel fence separation distance, and mitigation strategies on the rate of lateral flame spread and firebrand generation. The apparatus consisted of a single fence or parallel fence pair located on top of a mulch pan a distance away from and perpendicular to a target shed wall. A wind machine was placed behind the fence such that the flow it created was parallel to the fence. Bi-directional probes were placed 1.22 m (4 ft) upwind of the fence to capture the wind profile along the fence's leading edge. Tests were operated at fence-shed distances of 0 m, 0.91 m (3 ft), and 1.83 m (6 ft), and at wind speeds of 6 m/s (13.5 mph), 10 m/s (22.5 mph), and 14 m/s (31 mph). Parallel fence tests were conducted at fence separations of up to 91 cm (36 in). Most significantly, parallel fence configurations exhibited extreme fire behavior for all tested separation distances below 91 cm (36 in). This research will be used to influence codes and regulations related to fence construction and placement in WUI communities.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Andrew Seamone		**Award Number**	70NANB18H114
Academic Institution: University of Colorado, Boulder		**Major:** Civil Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate School for Aerospace Structures		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Structures Group		
NIST Research Advisor:	Dr. Travis Thonstad, Dr. Jonathan Weigand		
Title of Talk:	Structural Testing of Enhanced Steel Gravity Connections for the Mitigation of Disproportionate Collapse		

Abstract:
Steel gravity frames are commonly used in United States building construction practice, but they are potentially vulnerable to disproportionate collapse under column loss, as has been shown by recent experimental and analytical studies. To overcome these vulnerabilities, a new type of enhanced connection for steel gravity frames has been developed. These connections, which could be implemented either in new or existing structures, incorporate long-slotted steel plates that are welded to the column and bolted to the top and bottom flanges of the beam. To validate this new connection concept, long-slotted plate components were axially tested in a single-lapped bolted configuration to characterize their behavior and failure modes. Use of a load cell washer allowed for direct measurement of the tension in the bolt throughout testing. Tension in the connection bolt generally held until the plate and bolt connection reached bearing. Rapid tension loss in the connection bolt at bearing was predicted, but had not been previously measured before this series of testing, and the unique instrumentation of the experiment validated that the losses in connection bolt tension were indeed due to bearing with the lapped plates. Several types of slot geometries were tested while measurements of global and local strains and displacements helped characterize how the material reacted under stress. Quantifying the strengths of the different geometric slot configurations allows for the design of this connection detail to be optimized with predictable failure modes. This testing is the first step towards developing a design procedure so that the new connections can be used in practice. Results from the component tests will be used to validate previously developed computational models of a gravity frame assemblies. These models will be used to compare the performance of the enhanced steel gravity connections to conventional construction under a column loss scenario.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Esteban Segarra Martinez		**Award Number**	70NANB18H036
Academic Institution: Florida Polytechnic University		**Major:** Computer Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	I plan to start my PhD at a graduate university after completing my bachelor. Potentially work at a research facility in private industry or work in academia.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Dexterous Manipulation and Mobility Systems 735.13		
NIST Research Advisor:	Shelly Bagchi, Megan Zimmerman, and Jeremy Marvel		
Title of Talk:	Integration of Wearable Sensors into Virtual Reality (VR) and Augmented Reality (AR) Interfaces for Human-Robot Interaction (HRI)		

Abstract:
This presentation will demonstrate the use of an HRI interface to communicate with a virtual robot and the potential application towards a real-world industrial robot. Wearable virtual reality control devices, such as the Manus VR gloves, can mimic the movement of a real hand within a virtual environment. This type of control can be used to simplify tasks related to the training and control of an industrial robot. These tasks include situations where operators require precise or natural control over a device in teleoperation.

By using the Unity game engine, we can visualize the position and location of the Manus VR gloves as well as manipulate the virtual environment in a VR application. An API was developed for the Manus Gloves using the Manus SDK. In addition, C++ and C# interfaces were developed to export Manus VR data. Integration of the controls into NIST's Collaborative Robotic Programming Interface (CRPI) was performed but not utilized for the scope of this project.

Integrating the Manus gloves allows us to acquire sensory data referring to each of the individual fingers on a hand. By pairing this data with an attached VIVE tracker, we are able to precisely locate the user's hands in virtual space, and flexibly integrate hand-held controls inside a virtual environment.

The system performed as expected, with some minor complications in design due to unexpected difficulties in transmitting data from the virtual space to the real space. Real-time control over the virtual hand was obtained and displayed by controlling a virtual model of a UR5 robot arm.

Future work will concentrate on integration of the Manus gloves into a full VR robot interface, which can teleoperate a physical UR5 and an Allegro robot hand. The gloves will also be used as an interface for co-located HRI via AR.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Luis Serrano		**Award Number**	70NANB18H128
Academic Institution: Universidad del Turabo		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Graduated (June 2018)		
Future Plans (School/Career):	Pursue graduate studies in mechanical engineering.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Engineered Fire Safety Group		
NIST Research Advisor:	Dr. Randal McDermott		
Title of Talk:	Validation of Fire Dynamics Simulator		

Abstract:
The objective of this project is to validate NIST's Fire Dynamics Simulator (FDS) for the case of industrial flares. FDS is a computational fluid dynamics program for low speed, fire driven flows, developed to evaluate building performance with respect to fire growth, spread, detection, and suppression. As such, it is important to validate FDS and ensure the quality of the software. Although FDS has been validated for compartment fires and pool fires, it has yet to be validated for the case of industrial flares. Since the data on industrial flares is proprietary, two calibration burners designed at the National Fire Research Laboratory (NFRL) are used as surrogates, as they are similar to flares. Due to flare manufacturers' interest in the behavior of multiple flares with respect to flame dimensions, flame height is chosen as the validation target. A numerical study of the flame height obtained from the burners is performed using FDS. The flame heights are studied as a function of the burner's heat release rate. Another purpose of the project is to test FDS's capacity of accurately simulating complex geometries, as opposed to the block shaped objects that are usually used for the simulations. Three dimensional models of the NFRL burners are developed using a CAD software and exported to FDS. Test cases are run for a range of heat release rates and three different grid resolutions. Results from the burner models are compared to the video data from the NFRL calibration burners. Video data for flame height is manually extracted from NFRL recordings of the calibration burner experiments. As expected, the data indicates lower flame heights for the calibration burners fires compared to pool fires and sand burner fires.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Justin Sorra		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Work in the field for a few years before pursuing a graduate degree in Electrical Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, Mechanical Systems and Controls Group		
NIST Research Advisor:	Natascha Milesi-Ferretti & Michael Galler		
Title of Talk:	Laboratory Validation of HVAC-Cx Building Commissioning Software		

Abstract:
Heating, ventilation, and air conditioning (HVAC) systems commissioning is the process of analyzing the functionality of a new and existing HVAC systems. In many instances, the physical implementation of an HVAC system falls short of its theoretical design effectiveness and durability. Moreover, HVAC accounts for approximately 40% of total energy consumption in commercial buildings. Thus, HVAC commissioning can significantly reduce the cost and improve comfort of these buildings.

HVAC-Cx is a commissioning software tool for commissioning providers and building operators created by the National Institute of Standards and Technology (NIST) that provides ongoing commissioning and data analysis for commercial buildings. Data from various sensors throughout the HVAC system are imported, displayed graphically, and evaluated through a set of rules for malfunctioning or inefficient operations. When a rule is met, a fault is detected and the software provides a list of possible causes. Additionally, the Functional Performance Test Module (FPTM) is a feature of HVAC-Cx that allows real-time, active testing of HVAC system components and logic. Certain airflows, temperatures, or setpoints can be sent to the controllers to analyze how the components respond.

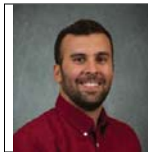
The purpose of my research is to test, improve, and utilize both the HVAC-Cx software and FPTM tools. We used HVAC-Cx to analyze actual data taken from a performing arts center at Montgomery College. With this data, we noticed significant operational and control logic errors that were evident long before the building operators were aware of any issues. Through this analysis, we could narrow the defective HVAC components and reduce the time and effort to debug the system malfunction. The FPTM was utilized in the lab to test high performance sequences of operation created by the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) for multi-zone variable-air-volume air handling units (VAV AHUs). Through this testing, we confirmed AHU responses to various system modes and situations, as well as error codes indicating improper operation. Finally, we added more custom options to test scripts and the HVAC environment to improve the FPTM's capabilities.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Xinran Sun		**Award Number**	70NANB18H135
Academic Institution: University of Michigan		**Major:** Industrial and Operations Engineering	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Pursuing a graduate degree and career in industrial and operations engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Information Modeling and Testing Group		
NIST Research Advisor:	Dr. Yan Lu		
Title of Talk:	Mass Customization Activity Modeling and Standards Landscape		

Abstract:
Today's customers want more personalized products and services that would better serve their needs. Hence, manufacturers are looking to expand their enterprises and product lines though embracing the tactic of offering special customization, with intensive customer involvement at every stage of product development lifecycle. However, enhanced integration of customer involvement in product development is relatively new and as such, no frame of reference has yet been defined. To help in defining a standards landscape for the mass customization manufacturing paradigm, an activity model for mass customization process has been developed. To do so, a literature review was first conducted. The current manufacturing activity model was assessed for identifying pre-identified terms and practices and the gaps of the model for the mass customization realm. Existing cases of businesses and organizations that provide mass customization were surveyed to serve as example structures. These cases, along with existing models of general manufacturing, were referenced to identify primary activities for a mass customization activity model. The various input, control, output, and mechanism components involved in the activities were then incorporated in to create a reference model for the manufacture of a mass customized product. The produced IDEF0 diagram helped support the identification of currently existing standards as well as standards gaps in mass customization manufacturing. These standards gaps can be examined in future studies to better define the mass customization standards landscape.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Cesar D. Tamayo Claro		**Award Number**	70NANB18H088
Academic Institution: Arizona State University		**Major:** Computer Systems Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing a career in Embedded Systems		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Life Cycle Group		
NIST Research Advisor:	William Z. Bernstein		
Title of Talk:	Incorporating Unit Manufacturing Process Models into Life Cycle Assessment Workflows		

Abstract:
Life-cycle Assessment (LCA) is a technique to assess environmental impacts associated with all the lifecycle stages of a product, process, or system, including raw material extraction, transportation, and end-of-life considerations, e.g., disposal or recycling. By quantifying all inputs and outputs of material and energy flows, LCA results can be used to make more environmentally conscious decisions about the specific scenario.

The goal of this work is to exploit the Unit Manufacturing Process (UMP) information model (ASTM E3012-16), to enable parametric environmental analysis of manufacturing systems without disrupting the traditional LCA workflow. The UMP concept allows for the consistent recording and exchanging of both physics-based and data-driven models, while labelling the analytical expressions with meta-data that provides domain-specific context, e.g. control parameters and machine conditions. In practice, when manufacturing-oriented LCAs are conducted, practitioners develop their own parametric models from scratch using various technologies, that are often difficult to reproduce and exchange. Introducing a consistent representation of manufacturing process models helps address this challenge.

Using a UMP model representing a simple vertical milling operation, we run simulations to instantiate a set of parameters and control variables and evaluate metrics of interests required to conduct an LCA. These results are validated against a case study from Wichita State University. We then generate an Ecospold file which can be imported into the LCA framework Brightway2. Once this step is completed, the model is linked to the Ecoinvent database, which contains thousands of inventory models allowing the LCA results to accurately reflect the entire life cycle of the product and its environmental impact.

This work constitutes a critical step for merging efforts related to process modeling and open-source frameworks that conduct LCAs, increasing the reproducibility, re-usability, validity and accuracy of LCA studies.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: John Walsh		**Award Number**	70NANB18153
Academic Institution:	University of Maryland, College Park	**Major:** Civil Engineering	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Graduating from the University of Maryland and pursuing a career in engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, HVAC&R Equipment Performance Group		
NIST Research Advisor:	Vance Payne		
Title of Talk:	Measuring Performance of an Airflow-Optimized Condensing Unit		

Abstract:
Finned-tube heat exchangers are primarily used for various air-cooling applications. Their main component is a bundle of several dozen connected tubes through which the desired refrigerant flows. The refrigerant must be routed so that the tubes exchange heat with the air as efficiently as possible, resulting in an overall high efficiency. As a result, the overall performance of the heat exchanger depends on the configuration of these tubes. To optimize the efficiency of the tube configuration, NIST has developed the Intelligent System for Heat Exchanger Design (ISHED), a generic algorithm (GA) approach that has determined that heat exchangers with optimized tube configurations for their airflow patterns can result in benefits including reduced size, cost, and refrigerant charge, as well as an increase in capacity and coefficient of performance (COP). This project monitors these improvements by comparing the performance of an airflow-optimized unit to the performance of a unit that has not been optimized. To accomplish this, Heat Pump Environmental Chambers were employed to test the performance of a condensing unit when connected to the optimized and standard units. The tests with the optimized heat exchanger (HX#1) provide the power and cooling capacity that the unit can supply for a range of evaporating saturation temperatures for various outdoor air conditions. After the testing of HX#1 is complete, it will be replaced with the standard heat exchanger (HX#2). Performance curves of each unit will be created and compared to one another to determine if there is a significant improvement due to the optimization of one of the units.

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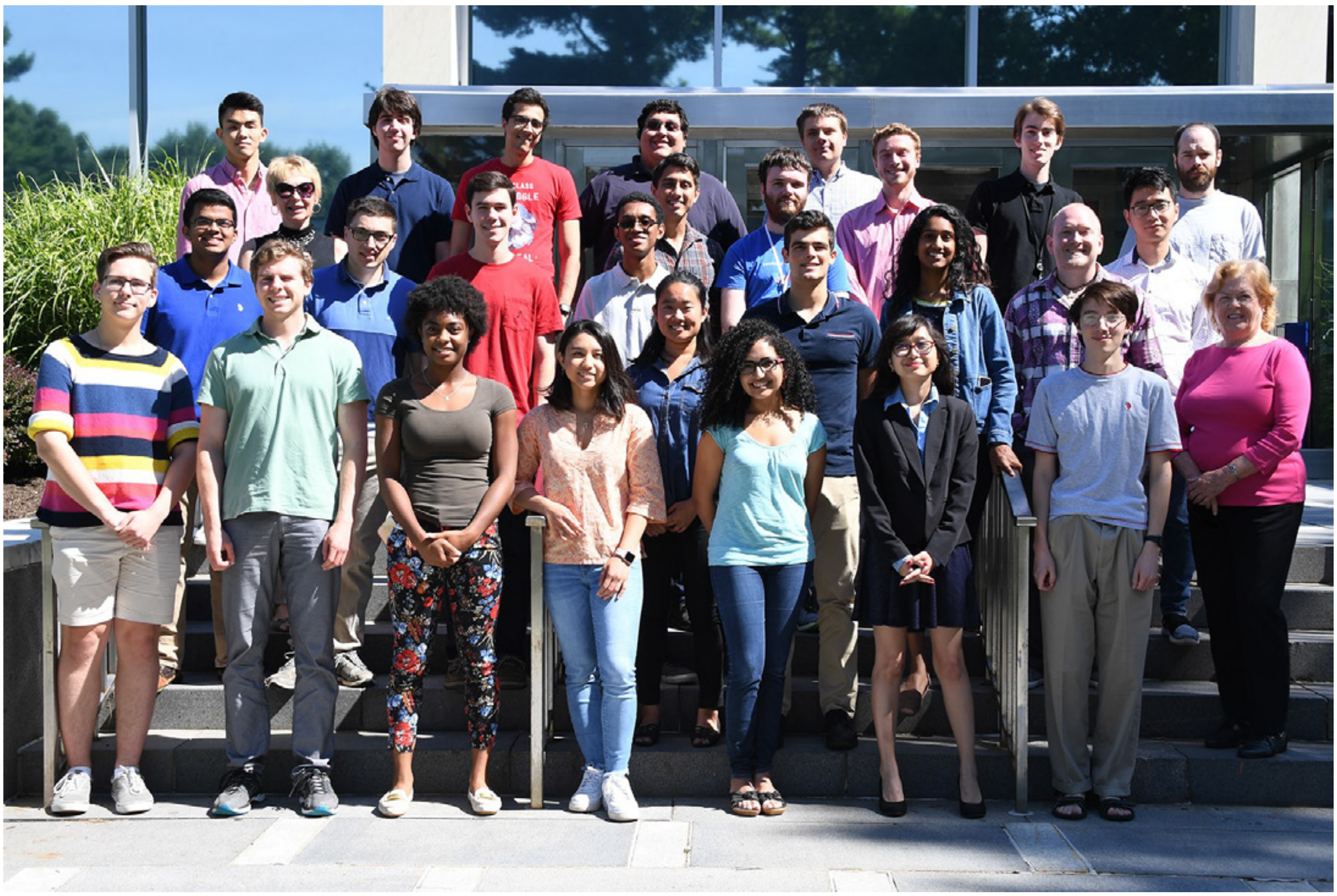


ITL

Last Name	First Name	Lab
Abraham	Sophia	ITL
Armstrong	Paul	ITL
Benz	Luke	ITL
Biggins	James	ITL
Boby	Kevin	ITL
Chiong	Golda Meir	ITL
Hailu	Surafel	ITL
Halam	Samantha	ITL
Klyuev	Arsen	ITL
Kupferschmid	Matthew	ITL
Li	Qing Hai	ITL
Li	Xiang	ITL
Malanoski	Aidan	ITL
Miller	David	ITL
Nachega	Nicholas	ITL
Nolan	John	ITL
Peake	Elijah	ITL
Perez	Felix	ITL
Pugh	Sydney	ITL
Roa	Michael	ITL
Shankar	Naveen	ITL
Steves	Paul	ITL
Vega Nogales	Alejandro	ITL
Vejalla	Varsha	ITL
Waysack	Joseph	ITL
Williams	Richard	ITL
Xiong	Xinyu	ITL
Zhu	Jesse	ITL
Zong	Kevin	ITL

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Sophia Abraham		**Award Number**	70NANB18H076
Academic Institution: University of South Florida		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate Studies in Computer Science		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Cryptographic Technology Group		
NIST Research Advisor:	Lawrence Bassham		
Title of Talk:	Authentication of RFID Communication with Wireless Identification and Sensing Platform (WISP)		

Abstract:

Radio Frequency Identification (RFID) is a manner of wireless communication that utilizes electromagnetic fields to identify and track tags. RFID systems consist of an antenna, reader and a tag. The RFID reader is a network connected device that utilizes radio frequency waves to relay signals that activate the tag which then transmits waves back to the antenna which is translated into data. RFID tags are highly constrained devices and the embedded microcontrollers pose difficulties in security challenges and vulnerabilities such as data integrity (ensuring transmitted data has not been altered or modified) due to smaller processors and fewer registers.

Modern encryption and hashing algorithms were designed to operate on general purpose computers with Central Processing Units that possess capabilities of implementing complex cryptographic algorithms. Due to the system constraints such as power deficits and limited memory allocation of the embedded microcontrollers in RFID tags, this project sought to utilize "lightweight" (work within the confines of electronics with limited resources) hashing and cryptographic algorithms to attenuate data integrity issues between RFID tags through Wireless Identification and Sensing Platforms (WISP) and a reader.

Encryption algorithms (e.g., ASCON, CHASKEY, etc) were implemented to provide authentication of the transmitted data between the WISP and the reader and resource utilization was examined. Though this project demonstrates authenticated communication between the WISP and reader on a simplified and small scale, similar approaches can be implemented to alleviate security concerns within complex RFID systems with numerous tags transmitting and receiving data.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

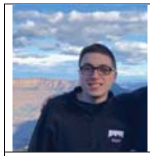
Name: Paul Armstrong		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Computer Science	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	I plan to graduate from the University of Maryland and pursue a career as a software engineer.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, High Performance Computing & Visualization Group		
NIST Research Advisor:	Wesley Griffin		
Title of Talk:	Virtual Reality as a tool for Cell Microscopy		

Abstract:

With Virtual Reality, separate perspectives are presented to each eye to create an illusion of depth. The perceived depth combined with six degrees of freedom produces a convincing immersion into a virtual space. This virtual space presents an interesting opportunity for visualization. My project is a continuation of an investigation into the practicality and usability of visualizing 3D confocal laser scanning microscope data in a virtual reality environment. We are visualizing the cell scaffold, cell growth, and pre-computed contact points where the scaffold meets the growth.

A-Frame, a WebVR framework built on THREE.js, allows us to create and distribute virtual reality scenes in a web browser. Using JavaScript, we create A-Frame components for navigating the scene, interacting with the scene, and marking poorly computed contact points. Our scene is compatible with the HTC Vive and the Oculus Rift.

We evaluate the effectiveness of two methods of marking the poorly computed contact points. The spherical marking method allows the user to create, stretch, and place an elliptical shape on the mesh while the rectangular marking method allows the user to paint a ribbon of rectangles on the mesh.



SURF Student Colloquium
NIST – Gaithersburg, MD
August 7-9, 2018

Name: Luke Benz		**Award Number**	70NANB18H072
Academic Institution: Yale University		**Major:** Applied Mathematics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	After graduation, I hope to work as a data scientist for a year or two before pursuing a PhD in statistics.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory Statistical Engineering Division Statistical Design, Analysis, & Modeling Group		
NIST Research Advisor:	Dr. Antonio Possolo		
Title of Talk:	Launch and Demonstration of the NIST Homogeneity Assessor		

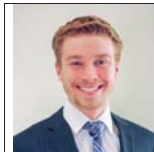
Abstract:
Assessing the homogeneity of candidate reference materials is a problem of great interest to many scientists at NIST and their colleagues at similar standards organizations around the world. The NIST Homogeneity Assessor (NIHOMA) is a newly developed application designed to aid scientists in assessing reference material homogeneity. NIHOMA serves to characterize the homogeneity of a candidate reference material for a particular measurand of interest based on replicated determinations of the value of the measurand in samples of the material.

The typical inputs for NIHOMA are either individual determinations made on aliquots of the material drawn from several containers, or summaries (for example, averages) of such determinations. In addition, the NIHOMA also requires that the sampling design be specified: for example, aliquots sampled from bottles, bottles sampled from boxes, etc. The goal is to compare the contributions that different sampling factors make to the overall dispersion of the measured values.

The NIHOMA uses a linear, Gaussian, random effects model, to estimate variance components attributable to the sampling factors. While statistically significant heterogeneity is commonly detected, in many applications a modicum of heterogeneity is acceptable, and the corresponding uncertainty component is recognized in the uncertainty budget for the estimate of the measurand, and taken into account.

In addition to estimating variance components and assessing their statistical significance, the NIHOMA also performs statistical tests and produces graphical displays that help users assess the adequacy of the underlying statistical model for their data and understand the sources of any heterogeneity that may be found.

This talk will feature a live demonstration of the NIHOMA, using a real dataset comprising measured values of the amount fractions of several compounds in a synthetic reference mixture designed to mimic natural gas.



SURF Student Colloquium
NIST – Gaithersburg, MD
August 7-9, 2018

Name: James Biggins		**Award Number**	70NANB18H153
Academic Institution: University of Maryland College Park		**Major:** Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Masters Degree in Computers Science and a career working in mixed reality development or software engineering		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, High Performance Computing and Visualization Group		
NIST Research Advisor:	Sanford Ressler		
Title of Talk:	Virtual Tours: Experiments in Monoscopic and Stereoscopic Virtual Reality		

Abstract:
Virtual Reality(VR) is a fast growing technology that is having an increasingly large impact in industries such as entertainment and research. People of all ages and interests can explore immersive, virtual environments. In addition, the creation of VR environments and systems closely resembles game development, and many game development systems can be adopted to create VR simulations.

Images in VR can be displayed monoscopically, so the images that surround the viewer appear in 2D, or stereoscopically, which creates a 3D effect. Although the creation of basic VR experiences has started to become more feasible to the general public, new technology has the ability to make such simulations more immersive.

Our project focuses on creating monoscopic and stereoscopic VR tours of NIST to give the public access to private spaces. Specifically, we experiment with a variety of 360 degree cameras to capture images and videos of different lab spaces. Next, we use the program Unity and the C# language to develop user interaction within these environments through a heads up display (HUD), informative videos, and text blurbs. This allows the user to learn about the area in which they are exploring. In addition, we explored the differences between stereo images and stereo video in a VR tour environment. Finally, by building these tours to be viewable on HTML web pages, we allow navigation by computer mouse controls, as well as most VR headsets.

Our research accomplished a step towards the goal of allowing NIST non-computer scientists to create their own virtual tours of their own labs. The web remains the most ubiquitous way of distributing information, and the recent support of VR devices with WebXR standards allows end users to simply go to a web address, a URL, and experience these scenes.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Kevin Boby		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Attending graduate school and starting a career in software development or cybersecurity.		
NIST Laboratory, Division, and Group:	Information Technology Lab, Software and Systems Division, Information Systems Group		
NIST Research Advisor:	Dr. Peter Bajcsy, Dr. Petre Manescu, Dr. Steve Feldman		
Title of Talk:	Automated Segmentation and Classification of Concrete Images		

Abstract:
Researchers from the Engineering Laboratory (EL) have been conducting experiments to understand the impact of alkali-silica reaction (ASR), one of the most serious causes of concrete degradation. NIST is currently developing measurements for quantifying ASR damage to better predict the relationship between loss of structural integrity/durability and to provide guidelines to regulatory agencies for meeting safe operations criteria. We must analyze ASR damage through 50 mm cylindrical cores drilled directly from larger structures over a long period of time, and under multiple operating conditions. Cores are imaged through scanning electron microscopy. Due to the volume of samples and image measurements, the processing challenge is approached by automating the information extraction.

We focused on the problem of automating the labelling of these images into regions that correspond to damage classes including cracking in the cement paste, and cracking and/or dissolution in complex aggregate components such as quartzite, etc. Our approach is to collect annotations for each class, create image masks defining annotated pixels, and then train a convolutional neural network (CNN). A collection of microscopy images was pre-processed into one 15635 x 15200 pixel image in a web image processing system. This image was annotated by the researchers from EL and then converted into multiple 256 x 256 images used to train the CNN, along with several pseudo-real images with known regions and class labels to test our CNN results.

Once the CNN is trained, we report accuracy of the model on the training and pseudo-real validation images. When the CNN model is applied to images without annotations, a visual inspection is used to assess the CNN model performance. All software in Python and Java has been deposited to a GitLab source code repository for future use.

CNN models can automate image segmentation tasks and achieve high accuracy as reported in the past literature. However, existing CNN architectures must be adjusted to individual tasks before they achieve high accuracy performance.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

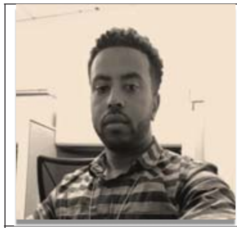
Name: Golda Meir Chiong		**Award Number**	70NANB18H113
Academic Institution: Towson University		**Major:** Computer Science	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a career in cybersecurity and attending graduate school		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Information Systems Group		
NIST Research Advisor:	Derek Juba		
Title of Talk:	Computational Reproducibility		

Abstract:
Reproducibility is an important yet often overlooked part of the research process. In computational sciences, differences in software and hardware can cause variations in floating-point results which can lead to differences in conclusions about one's data. Therefore, it is important to report the proper software and hardware specifications for research to be reproducible.

It is often unclear which computer system specifications will affect an experiment's results. Researchers often choose which specifications to include in an ad-hoc manner and sometimes even publish results without any specifications at all. It would be beneficial to researchers if there were a standard set of specifications to report.

As a step towards this goal, this project sought to pinpoint which compiler optimization flags and data type changes caused significant numerical variations in an image analysis test program used for the classification of cell colonies. This program examines the pixels within the image and computes a metric called entropy, which is later used to classify the colonies. Small variations in entropy would not change the classification, but drastic changes might.

To determine when reproducibility was broken, the entropy metric program was put through a test infrastructure called FLiT, which detects breaks in floating-point reproducibility caused by compiler optimizations and changes in floating-point data types. When breakages were detected, the next step was to examine whether or not the difference in the results affected the final classification of the cell colony. This provides an example of compiler optimizations which affect or do not affect the scientific conclusions of the study, which brings us one step closer to a standard set of specifications to report in computational research.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Surafel Hailu		**Award Number**	70NANB18H119
Academic Institution: University of District of Columbia		**Major:** Information Technology	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Advanced Network Technologies Division, Emerging Network Technologies Group.		
NIST Research Advisor:	Lotfi Benmohamed		
Title of Talk:	NDN-based IoT prototype deployment by using the ESP32 and Raspberry Pi platforms.		

Abstract:

The Current Internet is focused on new network architectures that can provide the much-needed scalability and network security. That's why the research is on the move to replace it with NDN Instead of requesting data using a server's IP address as it is the case today. Named Data Networking (NDN) is a new and a potential future Internet architecture that provides data-centric communication at the network layer and a much more flexible and intelligent network layer suitable for large data transfers. It is proposed recently as a clean-slate network architecture for future Internet, which no longer concentrates on "where" the information is located, but "what" the information (content) is needed. In NDN architecture communications, there is a consumer application which sends an Interest packet and a producer that replies with a Data packet that contains the content wanted by the consumer to satisfy those interests. This is achieved by matching Name and using forwarding states.

The part of my research and code implementation consists of applying C++ by using Arduino IDE platform. I am currently writing a code for a consumer to send an interest packets and a producer that replies with data packets as well as coding sensing application for the ESP. The overall goal of this project is to create and develop, inserting sensor data into repo-ng, sensing application on the ESP, connect to it from Arduino IDE, attach sensors to make them work, and Repo on the Pis is syncing each other. Once sensing server on the Pi that pulls data from the ESP and inserts into repo, we investigate whether repo insertion protocol works across one network hop, so that the ESP can insert in to the repo directly. Moreover, monitoring client application (web) after installing Web Server on pi so that the pi and ESP can communicate via Ethernet switch (or secondary WIFI interface in the future).

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August 7-9, 2018

Name: Samantha Halam		**Award Number**	70NANB18H078
Academic Institution: Fayetteville State University		**Major:** Computer Science and Computer Engineering (Double Major)	
Academic Standing (Sept. '18):	Transferring Senior at North Carolina State University		
Future Plans (School/Career):	Attend graduate school for Cybersecurity or work an entry-level job related to degree.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied Cybersecurity Division, National Initiative for Cybersecurity Education		
NIST Research Advisor:	Davina Pruitt-Mentle, Danielle Santos, Rodney Petersen		
Title of Talk:	Analyzing Cybersecurity in Academia Regarding the Botnet Report		

Abstract:

The U.S. employs nearly 770,000 people in cybersecurity positions, with approximately 302,000 current cybersecurity openings. It has been estimated that by 2022, there will be a 1.8 million global short of cybersecurity workers. The tremendous growth within the field over the past two decades has resulted in a substantial number of institutions of higher education (IHE) implementing a wide variety of academic approaches in an attempt to meet the growing demand for graduates and employees possessing skills in cybersecurity. This growth makes us ponder the question: what are the best models for teaching cybersecurity in IHE? This work delves deeper into one aspect of the report from the Department of Homeland Security (DHS) and Department of Commerce (DOC) on Enhancing the Resilience of the Internet and Communications Ecosystem Against Botnets and Other Automated, Distributed Threats to assess the scope and sufficiency of efforts to educate and train the American cybersecurity workforce of the future. The objective of my research is to analyze how top U.S. universities teach and/or integrate cybersecurity within their degree programs of study.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Arsen Klyuev		**Award Number**	70NANB18H093
Academic Institution: Johns Hopkins University		**Major:** Computer Science, Applied Math	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing a career in the tech industry before or after getting a master's degree in a computer science.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory Computer Security Division Security Components & Mechanisms Group		
NIST Research Advisor:	Richard Kuhn		
Title of Talk:	Using Block Matrices to Provide Erasure Capabilities to Blockchains Without Losing Integrity		

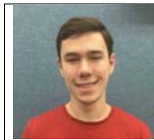
Abstract:

Blockchains are tamper evident and tamper resistant distributed digital ledger systems that normally do not have a central authority. They allow users to record transactions in a ledger public to their community, such that no transaction can be modified once it has been added to the ledger. However, the very immutability that makes blockchains secure also makes it impossible to remove any data in transactions and blocks once they have been added to the chain.

Growing privacy concerns and new privacy regulations, such as the European Union General Data Protection Regulation (GDPR), make the lack of ability to remove data from blockchains problematic. The GDPR, for example, requires that organizations make it possible to delete all information related to a specific individual at that person's request.

A block matrix is a newly designed data structure which could fix this problem. It provides integrity protection with erasure capability. The data structure itself, at its most basic level, is a matrix which stores the hashes of each of its rows and columns. Each "block" can be whatever the user wants it to be. It is structured such that it is possible to delete or modify the information in one block while still maintaining the integrity of all other blocks, as each block has at least 2 hashes ensuring its data is not tampered with.

By building blockchains on top of this data structure instead of the traditional hash-linked list, it would be possible to provide the security of traditional blockchains with the additional benefit of having the capability of deleting or modifying content in any block without losing integrity protection for other blocks. This has been implemented successfully in a basic demo, to provide functions that will be incorporated into other permissionless or permissioned blockchains, such as Multichain, in the future.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Matthew Kupferschmid		**Award Number**	70NANB18HO87
Academic Institution: Washington University in St Louis		**Major:** Mathematics	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	I plan to work as a data analyst when I graduate and then pursuing a PhD in statistics		
NIST Laboratory, Division, and Group:	Information Technology Lab, Information Access Division, Visualization and Usability Group		
NIST Research Advisor:	Yee-Yin Choong and Kristen Greene		
Title of Talk:	Understanding P@$$w0rds – password rule comprehension vs password generation		

Abstract:

Passwords are everywhere in our daily lives, from Twitter to a work or school email. Since we use passwords for almost everything, there is a common belief that creating more complex passwords can keep our information safer. These protections include mixing alphabets with special characters and numbers.

In this study, I looked into how well people actually understand terms like "special characters," "symbols," and "punctuation marks." To further understand how well people understand passwords requirements, NIST usability group conducted an experiment using an online platform – Amazon Mechanical Turk (mTurk). Ten different password generation rules were created in order to test the subjects' knowledge, with each subject randomly receiving a set of two rules to complete. I used data with over 10,000 passwords generated by subjects and analyzed many different features of passwords using R programming and Excel.

The results seemed to suggest that subjects generally comprehend what special characters are, but this doesn't seem to change their usage of special characters. Even when rules require special characters and the subjects are primed with character selection tasks, subjects repeated the same special characters (!,@,#) and some, such as tilde (~) and grave (`), are rarely used. There are some rules like punctuation and mathematical symbols that have a decreased percentage of correctly identified answers in the character selection.

These findings are important because they affect how we look at password requirements and password policy. With special characters in the requirements, people don't use them abundantly and often prefer certain special characters making the passwords predictable. Cybersecurity experts have suggested loosening password complexity requirements and encouraging users to create longer, more memorable passwords (NIST SP 800-63B Digital Identity Guidelines).

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Qing Hai Li		**Award Number**	70NANB18H073
Academic Institution: Wellesley College		**Major:** Mathematics & Physics	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Graduate studies in pure math.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied & Computational Mathematics Division, Mathematical Analysis & Modeling Group		
NIST Research Advisor:	Anthony Kearsley, Paul Patrone		
Title of Talk:	Analysis of Microfluidic Flow Rate Measurements		

Abstract:
Operation of microfluidic devices requires precise control over, and thereby measurement of, flow rates on the order of nL/min. At such scales, measurement signals are weak and require amplification. Current methods address this problem by relying on expensive microscopes, a detailed mathematical model of system geometry, and/or high resolution of the microfluidic device. However, such approaches are sensitive to uncertainties associated with device characterization, which propagate into final measurements.

Here, we expand on a recently proposed technique that overcomes such limitations by modelling flow rates in terms of the fluorescence intensity of dissolved fluorophores. In particular, this method relies solely on the observation that fluorescence efficiency, i.e. the measurement signal, is a one-to-one function of dosage, which is inversely proportional to flow rate. Critically, this property is robust: it holds irrespective of uncertainties in the device geometry and operating conditions. To further improve accuracy and facilitate uncertainty quantification, we argue that fluorescence efficiency is also a convex function of dosage. This allows us to apply powerful tools in convex optimisation to model the measurement signal, restrict the class of admissible fit-functions, and tighten uncertainty bounds.

We demonstrate convexity by showing that the second derivative of fluorophore concentration in dosage exists and is strictly positive. We recast this problem in terms of an existence proof of solutions to nonlinear integral equations, using Picard iteration. The proof does not require assumptions that compromise the robustness of the model. Experimental results confirm the validity of this approach.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Aidan Malanoski		**Award Number**	70NANB18H085
Academic Institution: Reed College		**Major:** Linguistics	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Information Technology Lab, Software and Systems Division		
NIST Research Advisor:	Sarala Padi, Eswaran Subrahmanian		
Title of Talk:	Combining syntactic parsing and vector semantics for keyphrase extraction for the root- and rule-based method		

Abstract:
The root- and rule-based method is a system for automatically generating standardized, domain-specific terminologies that can easily be customized for different information retrieval needs. However, the current terminology generator, Parmenides, makes no judgments about the relevance of terms to a document, instead selecting a linguistically defined set of phrases from a source text for processing. In this paper, we propose a new keyphrase extractor, VecRank. This extractor first uses word2vec to generate vectors that represent the semantic content of candidate keyphrases. It then applies PageRank, an algorithm for calculating the importance of nodes in a graph based on their relatedness to other nodes, to rank candidate keyphrases, from which we select the top candidates as the keyphrases for a document. This study involves two comparisons. First, we compare the phrases outputted by Parmenides alone with the phrases produced when the output of Parmenides is used as the input to VecRank. We then compare the output of the combination of Parmenides and VecRank with the output of VecRank without using Parmenides's output as its input. We generate keyphrases for a set of documents using each of the three extraction methods: the Parmenides extractor, VecRank, and their combination. Performance is evaluated using several metrics, including recall and precision, using author-assigned keyphrases as ground truth. Based on these results, we identify the extractor that best improves Parmenides's performance.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: David Miller		**Award Number**	70NANB18H153.
Academic Institution: University of Maryland, College Park		**Major:** Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Likely graduate school		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, Mathematical Modeling and Analysis Group		
NIST Research Advisor:	Michael Mascagni		
Title of Talk:	Stochastic Modeling of Round-off Errors in Scientific Computing		

Abstract:

Floating point numbers are used extensively in scientific computation, but arithmetic on them in most implementations, is inherently imprecise due to round-off, and while these errors are deterministic, they are unpredictable. Moreover, not all properties of real arithmetic hold; for instance, addition and multiplication are not associative or distributive. These kinds of issues can cause computations to misbehave. One example of this was previously found in a neuronal model consisting of a hundred neurons, with four differential equations per neuron. In the numerical solution, the reordering of what amounted to a dot product had significant impact on reproducibility.

To further investigate this, round-off error in the dot product was measured at each time step and then modeled statistically. Error due to round-off was calculated as the difference between a calculation with a hundred decimal digits of precision and the double-precision calculation, and then fit to various common distributions using the Kolmogorov-Smirnov goodness-of-fit test. After selection of an appropriate distribution, this was plugged back into a version of the simulation where the dot product was perturbed after computation. Finally, we used an ensemble of a hundred of these computations to determine consistency with the model, using the burst/episode times to test various modifications to the original model such as random shuffling (highlighting non-associativity), perturbations of initial conditions and of applied currents, and different compilers (running the same model). The resistance of a mitigation algorithm and extended precision to reordering was also examined.

We found that the round-off errors were relative to the value of the dot product, and that a normal distribution was the best fit. The consistency test found significant effects from large enough applied current changes (but not others), which is a desirable result, since the other changes are mathematically equivalent or minor.

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August 7-9, 2018

Name: Nicholas Biringingwa Nachega		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Working in Computer Systems Design and Artificial Intelligence		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Advanced Network Technologies Division (772), Internet and Scalable Systems Metrology Group (772.04)		
NIST Research Advisor:	Scott Rose		
Title of Talk:	A Test Transport Layer Security (TLS) Server for the DNSSEC Authentication Chain Extension		

Abstract:

Securing communications has been a focus for engineers working on the Internet since its inception. Protocols such as the Secure Sockets Layer (SSL) and its successor, the Transport Security Layer Security (TLS), were created to provide confidentiality and data integrity during communications between computer applications. Websites and web browsers, for example, use these protocols to secure passwords and other private data sent over the Internet.

The Internet Engineering Task Force (IETF), an international organization that promotes Internet standards, has put forward a draft proposal for an extension to the TLS protocol titled "A DANE Record and DNSSEC Authentication Chain Extension for TLS". This extension would allow TLS clients to perform Domain Name System (DNS)-based Authentication of Named Entities (DANE) validation of TLS server certificates without the need to perform DNS Security Extensions (DNSSEC) validation. This allows clients to use the DNS (with DNSSEC) information to perform domain validation of TLS certificates instead of (or in addition to) the traditional Certificate Authority (CA) infrastructure.

The purpose of this project is to develop a test TLS server that can return the DNSSEC authentication chain corresponding to its DANE record when it is requested by a TLS client. DNSSEC validation is not widely available for clients or may be too costly. The TLS server would need to perform a series of DNS queries in order to build the Domain Name System Security Extensions (DNSSEC) authentication chain that would allow a client to perform DNSSEC validation locally. The server would then return it to a TLS client when the new TLS extension is seen in a client handshake message.

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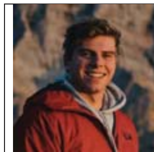
Name: John Nolan		**Award Number**	70NANB18H153
Academic Institution:	University of Maryland – College Park	**Major:** Mathematics	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Graduate School in Mathematics		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Cyber Infrastructure Group		
NIST Research Advisor:	Spencer Breiner (with additional supervision by Eswaran Subrahmanian and Blake Pollard)		
Title of Talk:	Compositional Approaches to Power Flow Problems		

Abstract:
Power flow problems, which require determining a valid set of (complex) powers and voltages in an electrical power network, arise frequently in power systems engineering. However, emerging technologies, including "distributed energy resources" such as solar panels and large rechargeable batteries, encourage a decentralized "smart" grid as opposed to the centralized architecture with which engineers are familiar. Power systems engineers face the challenge of modeling these resources and incorporating them into power flow problems. In addition, understanding the smart grid requires understanding the full space of possible solutions to power flow problems for a given network. Standard methods for solving power flow problems, such as Newton's method, return only one solution out of many possible solutions. To combat these challenges, we used techniques from compositional analysis, which studies how small systems combine into larger systems, and its formalization in category theory. We used categorical models to create databases modeling power flow problems and created programs to combine collections of distributed energy resources into easier-to-study constructs. In addition, we implemented a "pixel array" method based on compositional principles to identify all solutions to a power flow problem within a given region of the solution space. These tools will help power systems engineers prepare for the rising prevalence of distributed energy resources and demonstrate the usefulness of category theory and compositionality to real world engineering problems.



SURF Student Colloquium
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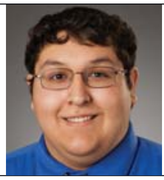
August 7-9, 2018

Name: Elijah Peake		**Award Number**	70NANB18H082
Academic Institution:	Middlebury College	**Major:** Mathematics, Computer Science	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Software Engineer for 2-3 years before pursuing higher education in Artificial Intelligence		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Information Access Division, Visualization and Usability Group		
NIST Research Advisor:	Michelle Steves		
Title of Talk:	Visualization Software to Analyze Password Policies		

Abstract:
Despite measures to replace passwords with other authentication methods, in many situations, traditional passwords remain unrivaled. Passwords are familiar to users, and they are convenient for organizations to implement. The language and complexity of password policies, however, is inconsistent. Policies are occasionally unclear and even contradictory, making it difficult for users to follow policy makers' intentions. The optimal intersection of security and policy usability remains unknown.

As a step to determine this intersection, NIST has developed a formal grammar for password policies. Translating all policies into the same language has allowed researchers to focus on the policies' meanings rather than the policy makers' writing styles. However, visualizing and exploring password policies were still difficult.

To help password policy researchers more easily explore password policies, we developed a piece of interactive visualization software with interface and technical domain requirements in mind. We used Python to parse policies because it handles language efficiently and D3.js, base JavaScript, HTML, and CSS for the visualization because they are flexible and allow for interactivity. The software allows researchers to import policies that have been translated to the formal grammar and immediately be presented with several key statistics and an updated, interactive visualization. Researchers can use this tool to explore how policies differ and are similar on an individual basis or even on much larger scales, such as how policies generally differ between major industry sectors. Using the tool, we have successfully compared policies of several industry sectors. The tool has provided us with insights through visualizations that were not previously possible with existing tools. Key to our exploratory analysis, the tool enables us to both visually and quantitatively explore the otherwise convoluted language of password policies.



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August 7-9, 2018

Name: Felix Perez		**Award Number**	70NANB18H142
Academic Institution: Texas Tech University		**Major:** Computer Science	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Attend graduate school to pursue a doctoral degree in Computer Science with focus in High-Performance Computing. After earning a PhD, work in academia to teach and continue HPC research. Alternatively, work at a national lab as a post-doc, or work as an industrial scientist in the private sector.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory (ITL), Applied & Computational Mathematics Division, Mathematical Analysis & Modeling Group		
NIST Research Advisor:	Anthony Kearsley		
Title of Talk:	Facilitating Development of Alternatives to Monoclonal Antibodies Through Readily-accessible Web Application Services		

Abstract:

Monoclonal antibodies are a class of biologic drugs sold in the pharmaceutical marketplace to treat several diseases, ranging from rheumatoid arthritis to certain kinds of cancers. In recent years, there has been exceptional growth in research and development of these drugs, which has yielded promising results of helping treat other diseases. Unfortunately, monoclonal antibodies are often prohibitively expensive to buy. However, due to recent patent expirations of innovator products, pharmaceutical companies can now begin developing generic alternatives to monoclonal antibodies. These potential generics, known as biosimilars, can make life-saving treatments more affordable by introducing competition into the marketplace.

To develop these biosimilars, an accurate experimental technique that can characterize the difference between the biologics and their biosimilar counterparts is required. Recently, it has been shown that two-dimensional nuclear magnetic resonance (NMR) spectroscopy is an excellent tool for characterizing the molecules of these drugs. Previously, analysis of NMR spectra has been limited to visual inspection and principal component analysis, which both lack an inherent measure of dissimilarity between the spectra. To facilitate the comparison of NMR spectra, the project team has developed a collection of dissimilarity measure-based techniques for classifying NMR spectra of monoclonal antibodies. These techniques rely on the interplay between an appropriate dissimilarity measure and a suitable unsupervised clustering algorithm.

The collection of techniques must then be widely accessible to researchers and industrial scientists for biosimilar development. Our team has chosen a web application approach to distribute the collection for the graphical user interface (GUI) capability of HTML pages with supplementary technologies such as JavaScript and CSS, the cross-platform portability of internet-based services, and the readily-accessible properties of hosted web pages. Through the design, development, and implementation of the web application, the collection becomes encoded into a format that is easily accessible, allowing for users to focus on the full utilization of the collection's computational capabilities. The final deliverable will enable researchers to classify NMR spectra of monoclonal antibodies from specified input and provide a novel visualization of the results.

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Name: Sydney Pugh		**Award Number**	70NANB18H096
Academic Institution: Loyola University Maryland		**Major:** Applied Mathematics and Computer Science	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue a Ph.D. in Applied Mathematics		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division		
NIST Research Advisor:	Rick Kuhn, Raghu Kacker, Mohammad S Raunak		
Title of Talk:	Developing Effective Test Strategies for Cryptographic Algorithm Implementations		

Abstract:

Cryptographic algorithms are essential for maintaining secure communication over any network. Due to their complexity, testing the implementations of such algorithms is very difficult because much of crypto algorithm complexity lies in bit manipulation and condition predicates, rather than program paths. Traditional testing strategies such as source code path coverage criteria based tests are generally ineffective. Cryptographic algorithms may be classified as "non-testable" programs [1] because they often lack a test oracle (i.e., a function that given a set of inputs, provides corresponding correct outputs) to verify that the implementation functions properly. Recent research applied a new testing strategy to cryptographic hash function implementations submitted to NIST's SHA-3 competition and found several bugs [2].

In this research, we turn to NIST's Post-Quantum Cryptography (PQC) Standardization process which aims to develop new quantum-resistant public-key cryptography standards. These cryptographic algorithms are designed to be secure against attacks from both quantum computers and classical computers. We applied a similar testing strategy to that applied to the SHA-3 implementations mentioned above. Furthermore, we developed new tests motivated by cryptographic properties specific to public-key encryption, key exchange, and digital signature schemes. Lastly, we developed tests motivated by the submission requirements imposed by NIST.

We implemented several tests. For example, we apply the Bit-Contribution Test developed by N. Mouha et al. to the PQC implementations to check that changes in the message yields changes in the encryption result. We developed the Bit-Verify Test for digital signature schemes to check that changes to the message after it has been signed result in unsuccessful signature verification. Our test strategy offers an effective way to test cryptographic algorithm implementations and catch potential bugs before these algorithms are deployed.

[1] E. J. Weyuker: On Testing Non-Testable Programs. Comput. J. 25(4): 465-470 (1982) https://doi.org/10.1093/comjnl/25.4.465
[2] N. Mouha, M. S. Raunak, D. R. Kuhn, and R. Kacker. 2018. Finding Bugs in Cryptographic Hash Function Implementations. IEEE Trans. Reliability: 15 pages (2018, to appear) https://dx.doi.org/10.1109/TR.2018.2847247

SURF Student Colloquium
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August 7-9, 2018

Name: Henry J Schmale	**Award Number** 70NANB18H098
Academic Institution: Millersville University of Pennsylvania	**Major:** Computer Science
Academic Standing (Sept. '18):	Senior @ Millersville University of Pennsylvania
Future Plans (School/Career):	I plan on going into either security research or reverse engineering of various software.
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied & Computational Mathematics Division, Mathematical Software Group
NIST Research Advisor:	Heman Gharibnejad, Barry Schneider
Title of Talk:	Benchmarking Numerical Approaches for Solving the Time-Dependent Schrodinger Equation in One Dimension

Abstract:
In molecular dynamics and quantum mechanical system modeling, solving the time-dependent Schrodinger equation (TDSE) in a reasonable time frame is very important. There are many numerical methods to solve the TDSE. Solving this equation requires stepping the solution forwards in time. Taking larger time steps allows for faster computation but at the cost of accuracy. This summer was spent measuring how much the accuracy cost versus the gained speed up using a model of 1-dimensional hydrogen atom.

Methods investigated include Lanczos with a 2nd and 4th order splitting, Crank-Nicholson over various gauges, and the Chebychev. We also investigate an iterative method for solving the TDSE. Timing was carried out on a standard Intel Xeon based desktop running CentOs 7. Both the wall clock time and the actual CPU time was measured. All code was implemented in Fortran compiled with the Intel Fortran Compiler using -03. The quality of the methods was measured by comparing probability plots in time.

We found that a group of implicit methods that allow taking larger time steps produce shorter run times with good accuracy. The hope is to find a method that combines the best features of each method in a fast iterative method. Computational implementations still do require optimization of the code, as stepping the solution forwards does not require keeping the results of the previous iterations in memory.

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Name: Naveen Shankar	**Award Number** 70NANB18H091
Academic Institution: Carnegie Mellon University	**Major:** Statistics and Machine Learning, Decision Science
Academic Standing (Sept. '18):	5th Year
Future Plans (School/Career):	Pursue a master's degree in machine learning
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Cryptographic Technology Group
NIST Research Advisor:	Kerry McKay
Title of Talk:	Using the Arduino for True Random Number Generation

Abstract:
Random numbers are of vital importance to society, as they form the backbone of nearly every modern encryption method. Most often, these random numbers are generated using a pseudorandom number generator - an algorithm which uses an initial value, called the seed, to deterministically produce strings of numbers which appear random. As such, keeping the seed secret is vital; if an attacker can guess the seed, they can determine all numbers produced by the pseudorandom number generator, and can break any corresponding encryptions. Hence, seeds must be truly random numbers, with sufficient bits of entropy (i.e. high enough uncertainty) that they are impossible to efficiently guess.

True random numbers are generated by entropy sources - devices which take readings from random physical phenomena, such as the time between two radioactive decay events, and optionally combine them with postprocessing methods to output random numbers. This project explores the efficacy of using the Arduino as an entropy source by measuring clock drift; measuring the discrepancies between the Arduino's two clock systems at the microsecond level.

Several postprocessing methods were tested, and each time a million numbers were generated. Entropy estimates were then obtained from these output streams according to the NIST standard. Even with NIST's conservative entropy estimation standard, the Arduino generated random numbers with 7.870 bits of entropy per 8 bits produced, or 98.38% of the total possible entropy. While the Arduino is still slower and produces slightly less random numbers than most top-tier true random number generators, it nevertheless offers a cheaper alternative to generating crypto-grade random numbers, and as such may have practical future applications.

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Name: Paul Steves		**Award Number**	70NANB18H089
Academic Institution: Washington College		**Major:** Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Pursuing a career in computer science		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Information Access Division, Visualization and Usability Group.		
NIST Research Advisor:	Kevin Mangold		
Title of Talk:	Augmented Reality Systems and Associated Metrics and Analytics		

Abstract:
While the Microsoft HoloLens is among the most known augmented reality technologies today, it is far from the only technology. Other augmented reality technologies exist primarily in a glasses format, while others, including the HoloLens, exist in a headset format. The structure desired for our research led us to believe that the headset format was most suited to our development needs with their increased abilities. The headsets we acquired came in the form of the Microsoft HoloLens and the Meta2 headset. Each headset we looked at provided their own technical challenges in the setup phase.

After a market survey assessing the current tools used to evaluate and measure interactions within virtual and augmented reality environments; we chose a software package provided by Cognitive3D. These tools record the most useful metrics for further analysis by usability and human-computer interaction experts. This data will be used to provide guidance to virtual and augmented reality developers on how to streamline their devices and digital environments. The reason for the project is to be better able to record and utilize data within an augmented reality environment with the purpose of facilitating emergency responder communication in emergency situations. My role in the project is extending the software provided by Cognitive3D to enable the use of custom events and metrics measurements.

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Name: Alejandro Salvador Vega Nogales		**Award Number**	70NANB18H127
Academic Institution: University of Puerto Rico, Rio Piedras		**Major:** Computer Science	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a research career starting with a Computer Science PhD. Very interested in a career in a federal research agency such as NIST, NOAA, a national laboratory, etc. In general, places where I can help advance our knowledge in some way and, at least tangentially, help the working class.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Information Systems Group		
NIST Research Advisor:	Timothy Blattner		
Title of Talk:	The HTGS Generator: A Tool for Generating Code for Multi-core systems		

Abstract:
The Hybrid Task Graph Scheduler (HTGS) is an API that increases programmer productivity with obtaining performance on systems with multiple CPUs. Unfortunately, using HTGS requires the programmer to write a significant amount of boilerplate code. This presentation introduces the HTGS Generator, which is a novel method and tool for designing parallel applications. This tool aims to improve the accessibility and productivity of implementing HTGS algorithms by having the programmer design their parallel application using the HTGS Generator's Graphical User Interface which constructs a task graph. The task graph is exported as a project and code is generated for each task and edge within the graph. These tasks and edges map directly into HTGS and are presented to the programmer with all of the boilerplate code automatically generated. The programmer only has to write the implementation of each Data Class container, Task execution, and data traversal strategy. The resulting implementation is a parallel application that receives all of the advantages of using HTGS and executes an algorithm across Multi-core systems.

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Name: Varsha Vejalla		**Award Number**	70NANB18H129
Academic Institution: University of Virginia		**Major:** Statistics/Economics	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Pursuing a career in economics and/or data science		
NIST Laboratory, Division, and Group:	Information Technology Lab; Statistical Engineering Division; Statistical Design, Analysis, and Modelling Group		
NIST Research Advisor:	Dr. Antonio Possolo		
Title of Talk:	Measuring Climate Change using Ice Cores		

Abstract:
Air bubbles trapped in polar ice can be retrieved from ice cores, providing a record of the earth's atmosphere and climate extending 800,000 years into the past. Estimates of atmospheric temperature (derived from oxygen and hydrogen isotope ratios) and relative abundances of greenhouse gases (GHGs) in prehistoric times provide a baseline against which changes in temperature and GHG abundances may be compared.

This research models changes in carbon dioxide, methane, and temperature over the past 800,000 years in Antarctica and connects them to recent measurements made by the National Oceanic and Atmospheric Administration's Global Monitoring Division. The variations in GHG abundances track temperature changes, aligning with known records of glacial and interglacial periods.

A local regression model (Loess) was fitted to measurements of atmospheric abundances of carbon dioxide and methane as a function of time, using observations from ice cores and modern measurements together. The concentrations of the two gases were also interpolated to fit an auto-regressive integrated moving average (ARIMA) model. Both the Loess and ARIMA models showed an increase in GHG concentrations since the Industrial Revolution to levels unseen in the past 800,000 years. Growth rates of methane and carbon dioxide concentrations were estimated using either interpolated data or local regression. Prior to the 17th century, growth rates fluctuated between -0.3 and 0.3 ppb/yr for methane and between -0.1 and 0.1 ppm/yr for carbon dioxide, but have since increased to post-industrial peak levels of 13 ppb/yr and 2 ppm/yr for methane and carbon dioxide respectively. While growth rates for carbon dioxide continue to climb, there has been a decline and subsequent stabilization in growth rates of methane since the 1980s, likely due to land use for agriculture leveling off.

The availability of data from ice cores has provided a way to analyze past glaciations and contextualize current shifts. However, additional proxy data will be necessary to extend climate records further into the past.

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Name: Joseph Jeffrey Waysack Jr.		**Award Number**	70NANB18H098
Academic Institution: Millersville University		**Major:** Computer Science	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	I plan to work in the field of augmented reality and pursue a master's degree along the way.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, High Performance Computing & Visualization Group		
NIST Research Advisor:	Judith Terrill & Steve Satterfield		
Title of Talk:	Monitoring Super Computer Simulations		

Abstract:

Supercomputer simulations are constantly running at NIST. Scientists running them, along with their collaborators, need to monitor these simulations, which can run for days, weeks, months, and longer. I have created a new program called MersivDB (Monitor, Explore, Review Simulations using Immersive Visualization Dashboard). This work extends Mersiv, a project that was started during SURF 2017. MersivDB allows users to search for a simulation of interest, filtered by characteristics such as the host computer, the simulation owner, and the simulation description. Upon finding a simulation within MersivDB, the user is then able to obtain up-to-date information, including its current state, plots of the latest output, and visual representations. Visualization can be displayed either on the user's workstation, or in ITL's immersive Visualization and Analysis Laboratory. This capability is designed to enable scientists to make sure that their simulations are running properly, and modify or terminate them if not.

The immersive laboratory at NIST, called the CAVE, uses 3 projectors and large screens forming the corner of a large, human-sized, box. This system immerses the user in 3D images and animations of their simulation. Included in the MersivDB interface is the ability for a user to view archived results from previous simulations as well as the latest results from currently running simulations.

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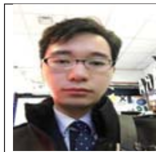
Name: Richard Williams Jr.		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Computer Engineering; Music	
Academic Standing (Sept. '18):	Undergraduate Senior		
Future Plans (School/Career):	Graduate school in Computer Science or a related field		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Cryptographic Technology Group		
NIST Research Advisor:	Dr. Kerry McKay		
Title of Talk:	Automatic Verification of Cryptographic Algorithms using SAW		

Abstract:

Cryptography has become increasingly important to all aspects computer security. Cryptographic systems are only secure when algorithms are implemented to align exactly with the standard that specifies the algorithm's details. In practice, algorithms can be implemented differently depending on performance constraints, so they must be tested extensively to verify that they meet their specifications. This presents a challenge because cryptographic security relies on having a very large key space. Thus, there is a need for automated tools that can mathematically verify an implementation to be correct in all cases. The Software Analysis Workbench (SAW) is a tool designed to formally prove properties of code using automated satisfiability solvers.

This research explored the effectiveness of using SAW to verify implementations of three symmetric ciphers: AES, RC4, and TripleDES. For each algorithm, several open source implementations in C were tested against the specification written in Cryptol. Proofs on complex functions like cryptographic algorithms were found to be a resource-intensive process for SAW on a desktop machine. The solver either took a large amount of time or did not terminate at all depending on the features of the specific implementation – for example, implementations designed for speed often had high memory usage and caused memory issues. However, breaking down each algorithm into smaller components showed more promising results. Another way to reduce the testing space is by forcing either the key or the plaintext to a fixed value, which greatly improved the efficiency in some instances. In addition, changing the compiler optimizations had no effect on SAW, which is a good sign for implementers. These conclusions show that SAW has potential for verifying cryptographic algorithms, but currently requires a large amount of computing resources to run efficiently.



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August 7-9, 2018

Name: Xinyu Xiong		**Award Number**	70NANB18H112
Academic Institution: The City College of New York		**Major:** Computer Science	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a career in software development field		
NIST Laboratory, Division, and Group:	Information technology lab, computer security division.		
NIST Research Advisor:	Vincent Hu		
Title of Talk:	Z Model for Next Generation Access Control (NGAC) Mechanism		

Abstract:

Next Generation Access Control (NGAC) is a fundamental reworking of traditional access control to meet the needs of the modern, distributed, interconnected enterprise. NGAC framework is flexible and can provide access control services for a number of different types of resources, accessed by a number of different types of applications and users. The design of NGAC is scalable, capable of supporting different types of policies simultaneously, and manageable in the face of changing technology, organizational restructuring, and increasing data volumes.

The Z notation is a formal specification language used for describing and modelling computing systems. It is targeted at the clear specification of computer programs and computer-based systems in general. Z is based on the standard mathematical notation used in axiomatic set theory, lambda calculus, and first-order predicate logic. All expressions in Z notation are typed, thereby avoiding some of the paradoxes of naive set theory. Z contains a standardized catalogue (called the mathematical toolkit) of commonly used mathematical functions and predicates, defined using Z itself. In this summer, My project is using Z model language to implement the NGAC model. After I build the model, I will verify/ and validate some critical -operational functions in of NGAC model.

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Name: Jesse Zhu		**Award Number**	70NANB18H068
Academic Institution: Cornell University		**Major:** Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Pursuing a career in software engineering		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Statistical Engineering Division, Statistical Design, Analysis, and Modeling Group		
NIST Research Advisor:	Dr. John Lu, Dr. Toni Litorja		
Title of Talk:	Use of lightfield cameras for capturing footwear impression: best practice and comparison		

Abstract:

The plenoptic camera was proposed at least 110 years ago but remains an underdeveloped technology which has the promise to change the future of image capturing. Unlike a traditional digital single-lens reflex (DSLR) that only captures 2D images, the plenoptic camera has an additional microlens array layer that contains hundreds of thousands of small hexagonal lenses, which captures the direction that light rays are traveling when they hit the sensor. Consequently, this allows for computation of 3D information and image refocusing after the images are taken. Computation plays a critical part in image measurement processing and is based partly on algorithms that reflect the optical physics used in traditional camera focusing. Our interest is to demonstrate application of the plenoptic camera in forensics, in particular, capturing footwear impressions whose 3D information is currently recovered by the tedious process of casting. The extra 3D ability of the plenoptic camera allows for the quantification of the unique pattern of each sole, including randomly acquired characteristics such as holes and tears. Currently, there are two main major manufacturers of this camera, Lytro and Raytrix. The goal of this study is to use Lytro and Raytrix cameras to collect footwear impressions under different scenarios and outside lighting to determine the best practices for lightfield cameras in measurement problems. This is evaluated through image processing and comparing the accuracy of the measurement results, including 2D and 3D depth.

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Name: Kevin Zong		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Computer Engineering	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Earning a master's degree in computer engineering		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, Computing and Communications Theory Group		
NIST Research Advisor:	Oliver Slattery, Lijun Ma		
Title of Talk:	Software for Single Photon Counter Interfacing and Data Analysis		

Abstract:

Quantum communication, in its current state, is limited in its applications due to the relatively short range that quantum signals can travel. Quantum repeaters can be implemented to extend the transmission distance of these signals; however, the implementation of a quantum repeater requires several crucial components. In this project, we will be focusing on the development of single photon entangled pair sources.

A clear indicator that a pair source is truly at the single photon level suitable for a quantum repeater is the temporal (time) correlation that exists between the two photons in a pair. A Time Correlation Single Photon Counting (TCSPC) device is used for the measurement and analysis of single photon detection events. For straight forward correlation measurements, the analysis tools provided by the device's software are sufficient. However, for more complicated or noisy correlation measurements, the device's standard software is not sufficient.

The goal of this project is to enable a more flexible analysis of correlation measurements in an automated and easy-to-use fashion. Using both LabVIEW and MATLAB, it is now possible to extract and save raw data from a TCSPC device and perform correlation analyses on a single photon pair source. The temporal correlation analysis will also provide valuable information that will help characterize the pair source in terms of linewidth and coherence time.

MML/NCNR

Last Name	First Name	Lab
Anderson	Eric	MML/NCNR_materials
Balto	Krista	MML/NCNR_materials
Behnert	Katie	MML/NCNR_materials
Bernier	Shannon	MML/NCNR_materials
Bhatnagar	Keshav	MML/NCNR_materials
Blitz	Jack	MML/NCNR_chem
Borgsmiller	Leah	MML/NCNR_materials
Brake	Alexis	MML/NCNR_materials
Brignac	Kayla	MML/NCNR_chem
Broerman	James	MML/NCNR_chem
Burni	Faraz	MML/NCNR_chem
Burrall	Hannah	MML/NCNR_materials
Cano	Alexa	MML/NCNR_materials
Cao	Tiffany	MML/NCNR_chem
Cavazos	Omar	MML/NCNR_materials
Clifford	Zachary	MML/NCNR_materials
Devers	Rachel	MML/NCNR_materials
Devorkin	Joshua	MML/NCNR_materials
Dharmadhikari	Kunal	MML/NCNR_chem
Fastow	Eli	MML/NCNR_materials
Filteau	Jeremy	MML/NCNR_chem
Finlay	Ethan	MML/NCNR_materials
Gonzalez	Shakira	MML/NCNR_chem
Hall	Steven	MML/NCNR_materials
Hamati	Michael	MML/NCNR_materials
Higgins	Brianna	MML/NCNR_chem
Horenberg	Allison	MML/NCNR_chem
Isaac	Samantha	MML/NCNR_materials
Janzen	Eli	MML/NCNR_materials

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Kant	Kamryn	MML/NCNR_materials
Keim	Klara	MML/NCNR_materials
Koehl	Julianna	MML/NCNR_chem
Kriz	Alison	MML/NCNR_materials
Martin	Sabrina	MML/NCNR_chem
McCright	Kevin	MML/NCNR_materials
Miller	Hallie	MML/NCNR_materials
Musteata	Elena	MML/NCNR_chem
Neves	Paul	MML/NCNR_materials
Ng	Daniel	MML/NCNR_materials
Nitschelm	Charlie	MML/NCNR_materials
Okusolubo	Temiloluwa	MML/NCNR_materials
Orenstein	Rachel	MML/NCNR_materials
Ott	Patrick	MML/NCNR_chem
Riedel	Zachary	MML/NCNR_materials
Riet	James	MML/NCNR_materials
Rodriguez Cardena	Viviana	MML/NCNR_materials
Roe	Emily	MML/NCNR_materials
Shah	Sejal	MML/NCNR_materials
Smith	Ryan	MML/NCNR_materials
Stakhovsky	Kirill	MML/NCNR_materials
Stemple	Carrie	MML/NCNR_materials
Strogen	Nicholas	MML/NCNR_materials
Sturek	Claire	MML/NCNR_chem
Suczewski	Gregory	MML/NCNR_materials
Swamykumar	Prateek	MML/NCNR_chem

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Tran	Ha	MML/NCNR_chem
Trowbridge	Julia	MML/NCNR_materials
Turner	MaKayla	MML/NCNR_materials
Underwood	Ryan	MML/NCNR_materials
Vincent	Galen	MML/NCNR_materials
Weiss	Abdullah	MML/NCNR_materials
Weyhmiller	Aubrie	MML/NCNR_materials
Wigham	Caleb	MML/NCNR_materials
Williams	Elijah	MML/NCNR_chem
Wilson	Abigail	MML/NCNR_materials
Winetrout	Jordan	MML/NCNR_materials
Wu	Sulan	MML/NCNR_materials
Yagodich	Julie	MML/NCNR_materials
Yoon	David	MML/NCNR_materials
Young	Candace	MML/NCNR_chem
Zambrotta	Ryan	MML/NCNR_materials

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August 7-9, 2018

Name: Eric Anderson		**Award Number**	70NANB18H075
Academic Institution: Northwestern University		**Major:** Materials Engineering & Physics	
Academic Standing :	Graduated from Northwestern		
Future Plans:	Graduate School for Physics		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Functional Polymers Group		
NIST Research Advisor:	Ryan Nieuwendaal		
Title of Talk:	ROMP Bottle Brush Polymer Structure Characterization via NMR and Computational Methods		

Abstract:

Recent polymerization techniques leveraging "click" chemistry and ring-opening metathesis polymerization (ROMP) have allowed for the synthesis of polymers with highly tailorable polymeric side chain chemistries, grafting densities, and molecular weights. These "bottle brush" copolymers have potential applications ranging from fuel cell electrolytes to microscale self-assembly, but are limited by uncertainty regarding the tacticities of their backbone units. Experimental determination of these tacticities via nuclear magnetic resonance (NMR) has proven difficult because of the complexity of the resulting spectra and the low chemical shift contrast between monomer units. Without a known molecular structure, further predictions regarding the properties of these copolymers could prove impossible.

Our aim is to determine the copolymer sequence distributions and cis/trans stereoisomeric populations for a set of bottle brush polymers consisting of a polynorbornene backbone and polylactic acid (PLA) or polyethylene oxide (PEO) side chains. We conducted a suite of 1-D and 2-D heteronuclear ^{1}H and ^{13}C NMR experiments, obtaining a complex spectrum of peaks resulting from variations in monomer couplings due to side chain distribution (ABA, BAA, etc.) and stereochemistry (trans-trans, trans-cis, etc.). *Ab initio* calculations were used to assign peaks and interpret the experimental results. Our assignment protocol will quantify the relative orientations of adjacent side chains and provide a molecular level picture of the contour of the polymer backbone, both of which are important for predicting rheological and transport properties. Our NMR protocol for these types of bottle brush polymers establishes a roadmap for characterizing and quantifying copolymers with increased architectural complexity.

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Name: Shannon Bernier		**Award Number**	70NANB18H034
Academic Institution: McDaniel College		**Major:** Chemistry and Physics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	To pursue a PhD in Physical Chemistry or Materials Science.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Chemical Process and Nuclear Measurements Group		
NIST Research Advisor:	Dr. Cary Presser		
Title of Talk:	Thermochemical analysis of SRM fuel blends using the laser-driven thermal reactor		

Abstract:

With today's ever-increasing variety of chemical compounds available for scientific and commercial use, there is a pressing need for ways to characterize and identify new or unknown compounds and mixtures. Common characterization techniques include spectroscopy, chromatography, and gravimetric analysis. While each is useful in its own way, no single method works perfectly for every type of compound. For this reason, expanding the characterization "toolbox" will always be an important area of research.

Our research has focused on the design and testing of a new characterization method used to investigate a substance's thermochemical behavior, referred to as the laser-driven thermal reactor (LDTR). The device seeks to mimic the rapid heating of typical combustion processes (such as those in an automobile engine) while maintaining high sensitivity. It uses laser heating to obtain signature thermograms (temperature vs. time plots), which can then be analyzed to provide information on the sample's heat release and mass change due to chemical reactions and/or phase changes.

We used the LDTR to test a range of NIST standard reference material (SRM) diesel/biodiesel blends, with two objectives. The first was to determine the total heat release of fuel mixtures, as an exploration of the LDTR's suitability as a renewable fuel screening tool. Our results proved comparable to literature values obtained via bomb calorimetry, thermal gravimetric analysis, and differential scanning calorimetry. The second goal, in collaboration with a chemometric research group here at NIST, was to test the device's ability to distinguish between different compounds and mixtures. We were able to demonstrate a relationship between observed thermal behavior and mixture concentration and also to automate our analysis protocol for estimating measurement repeatability. This analysis methodology will be used to further refine the LDTR as an identification and characterization tool in experiments with additional SRM fuels.

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August 7-9, 2018

Name: Keshav Bhatnagar		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Materials Science and Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Continuing school and pursuing a career in engineering consulting.		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Division 643, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group		
NIST Research Advisor:	Marcus Mendenhall		
Title of Talk:	Developing Operation Procedures for the Meca500 to Autonomously Swap Powder Samples in Divergent and Parallel Beam Diffractometers (DBD and PBD).		

Abstract:
The goal of my project is to increase the efficiency of data collection with two X-ray diffractometers. These diffractometers illuminate powder samples using X-rays, and the unique diffraction patterns that come from these samples are used to calibrate other diffractometers around the world. However, data can only be taken with these machines by manually changing the samples, restricting operation of this machine to the normal 9 AM - 5 PM work day. My project involves employing a high precision 6-axis industrial robot arm called the Meca500 to pick up samples from a 3D printed spinning sample-carrying carousel, as well as designing and 3D printing any parts deemed necessary to improve the divergent and parallel beam diffractometers. This would allow the robot to carefully load samples and place them in the DBD and PBD machines so that data can be taken 24 hours a day, significantly increasing the efficiency of taking calibration data. I began by using the computer aided design software OpenSCAD to design the carousel that the Meca500 would retrieve the previously loaded powder samples from. After 3D printing the final carousel as well as other parts to improve the functionality of the diffractometers (such as a 3D printed transmission bracket to stabilize a transmission used for a rotating part), I used the robotics software RoboDK to develop a code and a pattern for the Meca500 to follow when changing samples. The robot will be holding an electromagnet that can be turned on and off, which is what will be used to pick up the samples, since the powder is held in a magnetic metal base, however part of my project is to figure out a method to overcome the hysteresis caused by the electromagnet on the magnetic sample base. Although the code for the Meca500 is still in production, the result will increase the rate at which we will be able to take powder diffraction data for calibration of other x-ray diffractometers around the world.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Jack Blitz		**Award Number**	70NANB18H061
Academic Institution: Tulane University		**Major:** Neuroscience, Pre-Medicine	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing a career in medical research after receiving a M.D./PhD.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biomolecular Measurement Division, Applied Genetics Group		
NIST Research Advisor:	Megan Cleveland		
Title of Talk:	Droplet Digital PCR Assay Development of Clinical Reference Material for Epstein Barr Virus DNA		

Abstract:
Quantitative real-time PCR (qPCR) is commonly used for clinical testing of viral levels in immunosuppressed patients. Immunosuppressed patients (i.e. transplant recipients) must be regularly monitored by clinical testing laboratories to ensure proper immune system functioning. One problem with clinical testing currently, however, is the lack of standardized reference materials for many common viruses afflicting the immunosuppressed, such as Epstein Barr Virus (EBV), also known as Human Herpesvirus 4. The lack of standardized reference materials makes it difficult for clinical laboratories and medical professionals to compare results between laboratories for EBV testing and treatment. Using Droplet Digital PCR (ddPCR), DNA-based standards for the most common strain of EBV (Type A) were designed and subsequently tested for efficient PCR amplification. Understanding the sensitivity and specificity of the viral DNA is crucial in developing PCR assays that bind only to the intended target sequence because they can otherwise bind to multiple sites within the viral genome (resulting in inaccurate quantification) or bind to related viruses (leading to false positives). The large, approximately 171,000 nucleotide genome of the EBV Type A B95-8 strain makes this task difficult. Consequently, primers were designed with the aid of software, but primer design using computer software is by no means failsafe. Extensive laboratory testing of all the assays generated via the software was examined using digital droplet analysis to reveal the optimal annealing temperatures, lengths, and regions of the genome the primers are best suited for. It is this data that determines which EBV B95-8 assays are preferred over others and, ultimately, verifies which assays will be a strong candidate for a Standard Reference Material for clinical EBV testing. The assays were tested on purified EBV DNA from a cell line and the international standard for EBV. A NIST EBV reference material will be certified with ddPCR and used to calibrate secondary reference materials for qPCR.

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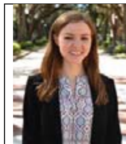
NIST – Gaithersburg, MD
August 7-9, 2018

Name: Leah Borgsmiller		**Award Number**	70NANB18H075
Academic Institution: Northwestern University		**Major:** Materials Science and Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Graduate school or working in industry as a materials scientist		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Material Science and Engineering Division, Polymers Processing Group		
NIST Research Advisor:	Dean DeLongchamp, Michael Heiber		
Title of Talk:	Impedance Photocurrent Device Analysis of Organic Photovoltaics		

Abstract:
Organic photovoltaics (OPVs) are promising in their ability to collect solar energy with devices that are lightweight, flexible, semi-transparent, and potentially cheaper to manufacture than their inorganic counterparts. However, for OPVs to be commercially competitive, further increases in power conversion efficiency must be obtained. Complicated relationships exist between device performance and the materials and device fabrication conditions used. In addition to complications arising from the numerous variables that impact device performance, not all measurement techniques produce accurate, reproducible data. To produce high quality data sets, a recently developed technique called impedance-photocurrent device analysis (IPDA) was set up and used in addition to more traditional current-voltage (J-V) curve analysis to characterize a variety of OPV devices. Full data on solar cell performance requires measurements to be taken under both light and dark conditions, and thus both the light source and dark boxes were carefully constructed to increase the reliability of the apparatus. As the first test case for the new measurement setup, OPV devices made of a BQR:PCBM donor-acceptor blend were selected. Both BQR and PCBM are small organic molecules that have previously demonstrated high power conversion efficiency. OPV devices were then fabricated with these materials using an industrially relevant blade-coating technique while varying the active layer thickness and thermal annealing temperature. These variables are known to impact active layer film morphology in this blend and the light absorption, which in turn can impact solar cell performance. These devices were then characterized using J-V measurements as well as the more refined IPDA technique to create a dataset of detailed device metrics. These metrics provide insight into the complex processing-structure-property relationships for the charge recombination and charge transport behavior in OPVs, which can be used by researchers in the future to further optimize device efficiency.



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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Alexis Brake		**Award Number**	70NANB18H131
Academic Institution: University of Florida		**Major:** Biomedical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Planning to attend a Ph.D./M.D. graduate program in pursuit of a career in medical research		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science Division, Security Technologies Group		
NIST Research Advisor:	Aaron Forster		
Title of Talk:	Ultrasound for materials research: Developing methods to quantify internal displacements in soft material tissue phantoms		

Abstract:
Protective equipment, including helmets and ballistic gear, is designed to prevent blunt injury during an impact. Innovation challenges, such as the National Football League Head Health Challenge series, show a critical need to develop better performing energy absorbing materials and better understand how materials can lower injury risk. A current roadblock is the current approach to material optimization that focuses on limiting maximum force or acceleration. This approach has been effective in preventing fracture in bone, but is limited in preventing soft tissue injury, which is driven by localized regions of high strain, like that in the brain. Currently, it is difficult to directly measure the strain of energy absorbing materials or soft tissue during an impact. Computer models are used to predict the distribution of force and strain during impact. Model validation is conducted by matching impact load vs. time response and predict the resulting strains. The ability to directly measure the strain in these materials during impact is a potential solution to improve model accuracy. Ultrasonic imaging is used in the medical field to evaluate structures, fluid velocity, and mechanical properties of soft tissues and recently, has been used to measure the jamming front propagation in shear-thickening solutions. This project developed and evaluated an ultrasound imaging technique for non-aqueous, non-linear elastic gel materials. The tissue phantoms were composed of styrene-ethylene-co-butylene-styrene (SEBS) triblock copolymers swollen in mineral oil. The stiffness of the phantom is controlled by varying the mass fraction of mineral oil, thus allowing it to represent different types of tissue. Internal strains and local velocities of tissue-simulating phantoms, subjected to compressive and puncture deformation at quasi-static rates, were measured. A 128-element ultrasonic transducer operating at 5 MHz was used to track the displacement of individual large particles (> 100 μm) as well as speckle patterns of smaller particles (< 100 μm). This presentation discusses the resolution and accuracy of the ultrasound measurement technique and potential implications for improving models of energy absorbing materials and tissues subjected to non-uniaxial impacts, such as those from sports injuries and ballistic events.

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August 7-9, 2018

Name: Kayla Brignac	**Award Number** 70NANB18H035
Academic Institution: University of Hawaii at Manoa	**Major:** Environmental Chemistry
Academic Standing (Sept. '18):	Senior
Future Plans (School/Career):	I plan to attend graduate school, earning a PhD in either environmental toxicology or materials chemistry with a research focus in plastic marine debris.
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Environmental Chemical Sciences Group
NIST Research Advisor:	Jennifer Lynch
Title of Talk:	Polymer Identification of Seafloor Plastics off the Coasts of the Hawaiian Islands

Abstract:
The plastic pollution crisis is now an internationally recognized threat to our environmental and public health. Many studies have focused on collections of beach, sea surface, and ingested plastics, but few have investigated the plastics that have sunk to the seafloor. This study is the first to identify the polymer composition of seafloor plastics found in the Hawaiian Islands. Three sample sites, two off the coast of Oahu and one off the coast of Maui, with dive depths less than 30 m were selected. A total of 216 samples were collected and analyzed using Fourier Transform infrared spectroscopy. The predominant compounds were nylon (n=59) and phthalates (n=23). Approximately 69% and 24% of the samples were sinking and floating polymers, respectively, while the remaining 7% were unable to be identified. The polymers that would have normally floated were either heavily biofouled or attached to a sinking component. A subset of samples (n=73) from beach plastics collected in 2017 was analyzed for multi-layer components to confirm accurate identification. Approximately 95% of the samples were confirmed to be mono-layer plastics. These results signify the importance of accounting for seafloor plastics as they comprise of mass-produced polymers and plasticizers not commonly found on beaches or the sea surface.

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August 7-9, 2018

Name: Adam Broerman	**Award Number** 70NANB18H114
Academic Institution: University of Colorado Boulder	**Major:** Chemical and Biological Engineering
Academic Standing (Sept. '18):	Junior
Future Plans (School/Career):	I plan to research the utilization of microbiology to improve current industrial and medical devices and processes, enhancing technology with biology. To gain experience in such research, I will pursue a Ph.D. in chemical engineering or bioengineering.
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biomolecular Measurement Division, Mass Spectrometry Data Center Group
NIST Research Advisor:	Arun Moorthy
Title of Talk:	A Computational Workflow for Annotating LC-MS Metabolomics Data from Biomanufacturing Cell Cultures

Abstract:

Metabolomics, the characterization of all metabolites (small molecule intermediates or products of an organism's metabolism) present in a sample to investigate correlations between their concentrations and observable cellular traits, has recently emerged as an invaluable tool for studying biological systems. Determining the identities and concentrations of biomarkers (molecules related to traits) gives insight into the current state of a biological system, informing, for example, actions to maintain its health or improve its product's yield and quality.

Liquid chromatography tandem-mass spectrometry (LC-MS/MS) is the analysis method of choice for elucidating structure and concentration of mixture components. Its superlative ability to scrutinize miniscule sample sizes and analyte concentrations without derivatization has enabled richer study of the complex metabolic processes occurring in biological systems. We use LC-MS/MS to identify all metabolites in extracts of Chinese Hamster Ovary (CHO) cells and media commonly used in drug bioproduction.

The fragmentation pattern captured in a mass spectrum manifests the unique fingerprint for its precursor molecule – potentially a biomarker. Regularly detecting the same fingerprint in different cell culture samples indicates that the corresponding precursor is likely a relevant metabolite. To ascertain whether a spectrum contains a valid fingerprint, we compute several metrics of spectral quality characteristic of spectra from real metabolites: their precursors must have been sufficiently fragmented, must have been mostly pure, and should have eluted from the chromatography column in a recognizable peak. We then group quality spectra that likely originated from the same compound (determined by the similarity of their fingerprints and behavior in the instrument) to obtain a comprehensive spectral profile for each metabolite. To assist reproducibility and uncertainty characterization, we are developing a software tool to automate these quality and similarity workflows. This tool will annotate and group similar spectra, facilitating mass-spectral library creation.

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August 7-9, 2018

Name: Faraz Ahmed Burni		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Will Pursue Masters in Chemical Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Security Technologies Group		
NIST Research Advisor:	Amanda Forster		
Title of Talk:	Ageing of Poly(p-phenylene terephthalamide) Fibers Used in Soft-Body Armor		

Abstract:
To improve the design and performance of soft-body armors, it is essential to understand the effects of ageing on the chemical and mechanical properties of materials used in body armor. This study is concerned with the long-term stability of poly(p-phenylene terephthalamide), or PPTA, which has been used extensively in body armor for many years. The investigation is carried out on both PPTA yarns and unidirectional (UD) laminates. These materials were exposed to a temperature of 70 °C, which approximates the maximum use temperature a typical armor may face during its lifetime (due to storage in a hot car, for example). Two humidity conditions were selected, 0 % RH and 76 % RH, to determine the potential role of humidity on the ageing of PPTA fibers. The samples were extracted at regular time intervals and are expected to be extracted until 20 weeks of exposure. Tensile tests were performed on the samples to determine the effect of ageing on the ultimate tensile strength and the failure strain. The results thus far (12 weeks) shows no significant signs of degradation, indicating PPTA fibers are very stable and does not degrade notably over the time interval and the exposed conditions. However, tensile tests on UD laminates at low extension rate of 1 mm/min, shows a reduction in tensile strength by about 6 %, which can be potentially attributed to the degradation of binder resin.

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Name: Tiffany Cao		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Bioengineering	
Academic Standing (Sept. '18):	Junior at University of Maryland, College Park		
Future Plans (School/Career):	Planning to pursue an MD-PhD program after graduation.		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science & Engineering Division, Polymers & Complex Fluids Group		
NIST Research Advisor:	Jeffrey Kim		
Title of Talk:	Characterization of electronic cigarette aerosol on hard surfaces		

Abstract:
Electronic-cigarettes (E-cigarettes) have been rapidly rising in popularity and have become the most used tobacco product among U.S. middle- and high-school students, surpassing combustible cigarettes. Currently, potential health risks of long-term vaping are not known and new products containing protonated nicotine and sweet flavor(s) are further complicating the issue. The aim of this study was to systematically characterize e-cigarette aerosol and determine the aerosol exposed surface changes that may have adverse biological implications. Reference e-liquids (no flavor, ethyl maltol, or menthol) with free-base or protonated nicotine were aerosolized using the Universal E-cigarette Testing Machine. We followed modified ISO smoking parameters which closely resemble human smoking topology. Collected aerosols were processed using an ultra-low temperature lyophilizer and visualized using Scanning Electron Microscopy. Surface changes were quantified by O'Toole-Kolter biofilm assay. Our aerosol analyses revealed that a 1.6 ohm heating element device with protonated nicotine generated aerosols of 10 - 50 micrometer diameter range, whereas a 0.2 ohm heating element device with free-base nicotine generated aerosols of ~1 micrometer diameter. Smoke from combustible cigarettes produced medium sized particles (5 - 10 micrometer) with a thick and irregular distribution. Our surface quantification data demonstrated that biofilm formation increased over time and was considerably higher in no flavor and menthol (with free-base and protonated nicotine) as compared to the control but not in e-liquids containing ethyl maltol. In conclusion, our data suggest that the resistance of heating elements and types of nicotine alter physio-chemical properties of aerosol and e-cigarette exposed surfaces may increase the risk of biofilm development.

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August 7-9, 2018

Name: Zachary Clifford		**Award Number**	70NANB18H101
Academic Institution:	University of Maryland, Baltimore County	**Major:** Chemistry	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	After obtaining a Bachelor's degree, I plan to attend graduate school to obtain a Ph.D. in chemistry. Then, I plan to become a research chemist.		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Nano Materials Research Group		
NIST Research Advisor:	Danielle Gorka		
Title of Talk:	Physical and Chemical Transformation of Silver Nanomaterial Containing Textiles After Use and Disposal		

Abstract:
In recent years, nanomaterials have been increasingly studied and used for their unique properties. Silver nanomaterials (AgNMs) have been incorporated into wound dressings because of their antimicrobial properties. However, the transformations that AgNMs undergo systematically throughout their life cycle are poorly understood. In this project, we studied the physical and chemical transformations to AgNM-containing textiles during simulated disposal conditions.

Here, a commercially available AgNM-containing wound dressing was studied. To understand the transformations that occurred during use and after disposal, wound dressings were exposed to synthetic freshwater or artificial landfill leachate (after disposal conditions) before and after exposure to synthetic sweat or simulated wound fluid (during use conditions). After being exposed to the desired set of conditions for varying duration, the wound dressing samples were characterized using a suite of analytical techniques.

During use and after disposal, the wound dressings underwent physical and chemical transformations. After exposure, there was a noticeable color change in the wound dressing. Scanning electron microscopy (SEM) images revealed the presence of crystals on the surface of the wound dressing after exposure to synthetic sweat. Energy dispersive x-ray spectroscopy (EDS) revealed that these crystals were mainly composed of silver and chloride. In contrast, wound dressing that was exposed to simulated wound fluid did not have large crystals on the surface. However, EDS determined that silver and chloride were both present. After exposure to disposal conditions, SEM images showed increased granularity in the silver layer on the surface of the wound dressing. EDS found that the wound dressing contained mostly silver with trace chloride signatures. Wound dressings that were exposed to both during use conditions and after disposal conditions will also be discussed.

This project revealed that AgNM-containing wound dressings undergo transformations during use and after disposal. Future studies will look at how these transformations affect the antimicrobial properties of the wound dressing. The results of this project will allow manufacturers and regulators make better decisions about design, use, and disposal of AgNM-containing textiles.

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August 7-9, 2018

Name: Rachel Devers		**Award Number**	70NANB18H153
Academic Institution:	University of Maryland, College Park	**Electrical Engineering**	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue an advanced degree in computer science, data science or information science		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science and Engineering Division and the Office of Data and Informatics, Data Sciences Group		
NIST Research Advisor:	June Lau and Gretchen Greene		
Title of Talk:	The development of an electron microscopy dossier		

Abstract:
The Electron Microscopy Nexus is a network of 7 microscopes operated by scientists in MML for materials science research. The current data infrastructure for the Nexus serves primarily as a waypoint (and little else) for data generated by the instruments on its way to researchers' desktops. Additionally, current data management efforts require substantial manual effort to capture, record, and effectively store data from experiments and lack the capabilities to readily parse who collected data, using which instrument, on what sample and why. Ultimately, current practices are also incompatible with FAIR data principles (findable, accessible, interoperable and reproducible data). We propose modernizing this system by creating an automated wiki-style dossier of microscopy session data and metadata to enable materials related electron microscopy data discovery, curation, and long-term management.

The full information set that imparts meaning to a particular microscopy session may include sample information, session notes, observations, and any subsequent data/image analysis or spectrum. This information set often contains rich information, in a variety of structures and formats, all captured and stored in various locations, making long term retention of the narrative and the associated datasets non-trivial. Fortunately, such experimental context and crucial metadata can often be found in digital locations. In this project we outlined and took the first step towards developing a microscopy dossier, by mining existing digital data sources such as electronic lab notebooks (ELN's), online tool reservation calendars, and raw instrument-generated image metadata.

We sought to tackle the heterogenous and dissociative nature of these sets of information by developing an XML schema, as well as scripts to automatically populate XML files using metadata collected from the aforementioned digital resources. Using NIST's Configurable Data Curation System (formerly known as MDCS) as our dossiers' backbone, the generated XML descriptions are translated using XSLT stylesheets, so that data of diverse types (images, text notes, tabular data, etc.) can be optimally viewed by researchers in a web browser. The end goal of this project is to make electron microscopy data and metadata more searchable, relatable, and ultimately reusable, which will in turn enable more rapid material discoveries. Our solution promotes materials-related electron microscopy data discovery, curation, and long-term management.

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August 7-9, 2018

Name: Kunal Dharmadhikari		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Bioengineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	After obtaining my undergraduate degree, I plan on pursuing a Masters with a concentration in Biomedical computation. I hope to develop technologies that solve medical and health related problems.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biomolecular Measurement Division, Biomolecular Structure and function Group		
NIST Research Advisor:	Dr. Christina Bergonzo and Dr. Jennifer Tullman		
Title of Talk:	Structural Basis of ClpS Specificity Probed by Molecular Dynamics Simulations		

Abstract:

ClpS is a small protein which is currently being developed as a probe for detecting specific N-terminal amino acids of peptides. However, in order for ClpS to be used in this manner, it is extremely important to understand the structural reasons for how and why ClpS recognizes specific residues

To understand the specificity of the recognition mechanism of ClpS, simulations were conducted on wild-type (WT) ClpS and ClpS mutants. Once data was obtained from these simulations, several methods of analysis were used to conduct calculations for the binding free energies per residue.

Specificity of the WT ClpS was heavily influenced by lower electrostatic contribution to the solvation free energy. The binding free energies have shown that ClpS has higher affinities for Phe in comparison to Tyr and Trp, due to lower electrostatic contributions to the solvation free energy. The PROSS mutant (ClpS with 9 mutated residues in the same system) has shown to have a similar estimated binding free energy as the highly favored WT. Two mutations, V22E and E64Q, had the greatest change in contributions to electrostatic energy. Therefore ClpS, with these two mutations, can be predicted to be able to stabilize binding for different N-terminal amino acid combinations. The methods used to conduct this study are transferable to enable engineering artificial protein-interaction networks and are useful in drug delivery problems.

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August 7-9, 2018

Name: Eli Fastow		**Award Number**	70NANB18H153
Academic Institution: University of Maryland College Park		**Major:** Material Science Engineering	
Academic Standing (Sept. '18):	Rising Junior		
Future Plans (School/Career):	Attend graduate school for a doctoral degree		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science and Engineering Division, Functional Nanostructured Materials Group		
NIST Research Advisor:	Dr. Cindi Dennis		
Title of Talk:	Annealing Temperature and Underlayer Effects on Perpendicular Magnetic Anisotropy Energy of $Co_{20}Fe_{60}B_{20}$/MgO		

Abstract:

Materials that exhibit magnetic anisotropy (K), or energy required to rotate the direction of magnetization 180 degrees, enable storage of data as either 0 or 1 depending on direction of magnetization if K does not equal 0. Magnetic random access memory (MRAM), a type of magnetic data storage, is a candidate for next generation storage technology given its high speed, low power consumption, long endurance, and high information density. Existing materials used in MRAM exhibit parallel anisotropy, where the preferred direction of magnetization lies in the plane, or parallel to the surface, of the magnetic thin film. However, materials where the preferred axis of magnetization lies normal to the surface of the magnetic thin film, called perpendicular magnetic anisotropy (PMA), potentially exhibit higher information density and better writability than those with parallel anisotropy. Magnetization typically prefers a direction in the plane of a device, requiring materials engineering to achieve PMA. This work examines the effect of an underlayer that seeds growth of the magnetic material and its annealing temperature on the PMA. The device consists of a stack with the structure SiO2/underlayer/Co20Fe60B20/MgO formed through sputter depostion. We analyze a broad survey of underlayers (selected from Ti, V, Cr, Zr, Mo, Ru, Rh, Ag, Hf, Ta, W, Re, Os, Ir, Pt, and Au) and the effects of their annealing temperatures (315, 350, 375, and 400 °C) on the magnetic anisotropy. We measured PMA with torque magnetometry, or magnetization at a constant field as a function of field angle, and hysteresis loops, or magnetization of the material as a function of external field. Hysteresis loops, measured parallel and perpendicular to the plane of the device, and torque curves allow for the identification of the preferred orientation of magnetization and anisotropy constants.

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August 7-9, 2018

Name: Jeremy Filteau		**Award Number**	70NANB18H065
Academic Institution: Worcester Polytechnic Institute		**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Graduate Student at University of Washington		
Future Plans (School/Career):	Pursuing a PhD in Chemical Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biomolecular Measurement Division, Bioprocess Measurements Group		
NIST Research Advisor:	Dr. Wyatt Vreeland		
Title of Talk:	Mechanism behind rapid protein aggregation by novel azide-assisted chemistry		

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 biologics market projected to reach $500 billion (US) in sales per year by 2024. Protein-based drugs are particularly susceptible to chemical and physical degradation causing these drugs to aggregate, where multiple protein molecules assemble in an uncontrolled and undesirable fashion into large particles. The resulting aggregated therapeutic can cause negative effects, including embolisms, renal impairment, and immunogenic responses. NIST is producing protein aggregates in the submicron size range to harmonize measurement across various instrumentation platforms. Thermal stress in buffers containing the anion azide causes rapid aggregation, drastically reducing incubation time relative to native buffer (those without azide). The resulting azide-assisted aggregates are separated via Asymmetric Flow Field Flow Fractionation (AF4), and characterized in-line with Multi Angle Light Scattering (MALS), and off-line with Mass Spectrometry (LC-MS). We demonstrate this procedure with bovine serum albumin (NIST SRM 927f), where the resultant mixture consists of monomeric protein and aggregated protein in various ratios. The ability of AF4 to separate the aggregated protein from residual monomeric protein allows for accurate determination of the amount of protein that has been aggregated as a function of stress conditions. When combined with the abilities of MALS and LC-MS to determine molar mass and protein structure, respectively, the mechanism behind azide-assisted aggregation can be elucidated. This technique should be directly applicable to more complex and specific proteins.

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August 7-9, 2018

Name: Ethan Finlay		**Award Number**	70NANB18H050
Academic Institution: Appalachian State University		**Major:** Physics and Chemistry	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue a Ph.D in Physics or Organic Chemistry and either go into research or become a professor		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group		
NIST Research Advisor:	Jirun Sun		
Title of Talk:	Exploring Clinically Relevant Approaches to Reduce Polymerization Stress of Dental Composites		

Abstract:

Polymerization stress is a major concern for dental resin composites due to its catastrophic effects that may lead to tooth fracture and secondary caries. In this project, I will introduce two approaches to reduce polymerization stress: 1) using a monomer mixture containing an ether-based hydrolytically stable monomer, triethyleneglycol divinylbenzyl ether (TEG-DVBE), which can be photo-polymerized with an ester-based monomer, e.g., urethane dimethacrylate (UDMA) during which follows composition-controlled co-polymerization kinetics, and 2) using a novel cationic initiator that has antimicrobial potentials. The real-time polymerization stress and degree of vinyl conversion were evaluated simultaneously using a self-calibrated VRC and NIST-developed setup with a tensometer and near infrared spectrometer. An ester-based traditional resin composite, which contains the resins bis-phenol-A-glycidyl-dimethacrylate (BisGMA) and triethylene glycol dimethacrylate (TEGDMA) with camphorquinone/amine initiators (CQ/amine) and 75 % mass fraction of fillers, was used as a control. Previously determined effective molar ratios of all monomer mixtures were used to maximize experimental results. The individual and combined effects of the new resin mixture and the new initiator to the polymerization stress of resin composites were assessed. As reported previously, the photo-copolymerization of this monomer mixture is an azeotropic copolymerization when CQ4E is used as an initiator. The composites made of this resin mixture have equivalent or better chemical, physical, and mechanical performances than the controls. In addition, the new cationic initiator is also an antibacterial agent that may selectively inhibit the growth of acid-producing bacteria, such as S. mutans. It was used in addition to CQ/amine. All the new compositions of resin composites generated less stress than the controls. This and other advantages of using the new resin and initiator together will be discussed. In summary, these results suggest that the new compositions have significant improvements in performance that provide great potential to replace current dental resin composites.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Shakira González		**Award Number**	70NANB18H127
Academic Institution: University of Puerto Rico at Arecibo		**Major:** Medical Microbiology	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Planning to attend a M.D./Ph.D. graduate program and become an aerospace medicine specialist/flight surgeon.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biosystems and Biomaterials Division, Bioassay Methods Group		
NIST Research Advisor:	Paul DeRose		
Title of Talk:	Characterization of Fluorescent Dyes for the Assignment of Fluorescence Intensity to Calibration Microspheres for Flow Cytometry		

Abstract:

Flow cytometry is a technique used to count, differentiate and separate different types of cells present in biological samples. It is an essential tool used in immunological research, disease diagnostics and clinical treatments. In addition to analyzing a cell's characteristics, a flow cytometer can detect emitted light from excited fluorescent molecules, such as fluorescently-labeled antibodies. Fluorescence intensities of cells measured by flow cytometers need to be more reproducible between instruments, laboratories and over time to improve patient outcomes. In order to achieve this, it is necessary to calibrate the fluorescence signal of flow cytometers using calibration microspheres with known fluorescence intensities. The equivalent number of reference fluorophores (ERF), implemented by the flow cytometer community with the help of NIST, gives the number of reference fluorophores in solution which produces the same fluorescence signal as a single dyed microsphere. It includes information about the excitation wavelength and emission spectral range, which allows the ERF to be used as a scale of fluorescence intensity. NIST has developed standard reference material (SRM 1934) to support the calibration microsphere's fluorescent signal in terms of ERF. The SRM 1934 includes four solutions of fluorophore: Allophycocyanin (APC), Coumarin 30, Fluorescein and Nile Red.

For complex biological assays, thirty or more fluorescence channels with as many as six excitation wavelengths and six or more different emission filters may be used. More reference solutions beyond those in SRM 1934 are required to put all these fluorescence channels on ERF scales. The goal of this research is to identify new reference fluorophore candidates. High-Performance Liquid Chromatography (HPLC) and NMR were used to determine the purity of the following candidate dyes: Pacific Orange, Alexa Flour 700® and Alexa Flour 750®. Once the purity is known, gravimetry can be used to make up reference solutions with known concentrations of the sample constituents. Absorbance and fluorescence spectra of these candidate dye solutions were also measured on a spectrophotometer and fluorescence spectrometer, respectively, as complementary techniques to HPLC. The dyes were found to be of sufficiently high purity to be used as reference fluorophores for ERF assignments of calibration microspheres.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Steven Hall		**Award Number**	70NANB18H141
Academic Institution: Clemson University		**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Graduate Student at Clemson University		
Future Plans (School/Career):	Pursue a PhD in chemical engineering and a career in independent research.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Research Group		
NIST Research Advisor:	Harold Hatch		
Title of Talk:	Charge Expanded Ensemble for Efficient Sampling of Ionic Systems		

Abstract:

Ionic liquids show potential as tunable high-performance chemicals and industrial solvents. As such, there is interest in predicting and understanding their properties through molecular simulation. Monte Carlo simulations in the grand canonical ensemble are a convenient way to predict the vapor-liquid equilibrium properties of ionic liquids. Because natural systems are charge-neutral in the thermodynamic limit, conventional simulations of ionic systems with periodic boundaries insert and delete neutral sets of ions. At low temperatures and liquid densities, this causes calculations to become computationally expensive due to difficulties in configurational sampling. We introduce a new expanded ensemble approach that allows ionic liquid simulations to sample the neutral states of interest by efficiently inserting individual ions that are neutralized using a delocalized background charge as implemented in existing electrostatic energy calculation methods. Flat histogram Monte Carlo methods are then used to reconstruct the thermodynamic properties of the neutral states. We first demonstrate that the vapor-liquid equilibrium properties of a binary square-well fluid obtained with the conventional and expanded ensemble insertion methods are equivalent. We then calculate the vapor-liquid phase diagram for monovalent charged hard spheres. At liquid densities, we observe an order of magnitude increase in the efficiency. This method can potentially be extended to more complex molecular ionic liquids and other ionic systems to more efficiently screen novel chemicals for their properties.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Michael Sargon Hamati		**Award Number**	70NANB18H062
Academic Institution: Columbia University in the City of New York		**Major:** Materials Science & Engineering	
Academic Standing (Sept. '18):	Graduated Senior		
Future Plans (School/Career):	Applying to graduate school		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group		
NIST Research Advisor:	Dr. Winnie Wong-Ng		
Title of Talk:	Synthesis and Characterization of Monodisperse Cerium Oxide Nanomaterials		

Abstract:

Nano-sized CeO_2 (nanoceria) is known to have important industrial applications, including vehicle exhaust catalysis, ion conductors in solid oxide fuel cells, the production of hydrogen from water, and nanomedicine. To increase the efficacy and use of nanoceria in these applications, their size dependent chemical and physical properties must be accurately measured. A series of CeO_2 monodisperse nano-materials with different sizes (between 10 nm and 1 µm) was successfully prepared using a novel solution-phase synthesis method. In this presentation, we will describe our synthesis technique and discuss the results of chemical and physical property characterization, including those obtained by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), neutron diffraction, and thermal gravimetric analysis (TGA). Temperature dependent heat capacity was also measured using a Physical Property Measurement System (PPMS). In the time remaining, we will describe our future work.

SURF Student Colloquium

NIST – Gaithersburg, MD

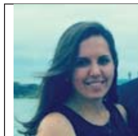
August 7-9, 2018

Name: Brianna Higgins		**Award Number**	70NANB18H053
Academic Institution: Hood College		**Major:** Biochemistry	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Material Measurements Laboratory, Materials Science and Engineering Division, Functional Polymers Group		
NIST Research Advisor:	Dr. Jeremiah Woodcock		
Title of Talk:	Design and synthesis of mechano-responsive fluorophores for localized visualization of damage in polymer composites		

Abstract:

The integrity of composite materials is essential due to extensive public reliance on the constructional durability of structures such as airplane wings, wind turbine blades, composite rebar, and composite pressure vessels. Mechanophores, sometimes called "mechanochromophores," have the ability to fluoresce in response to mechanical stimuli such as cracks and tensile strain when incorporated into polymers. Current mechanophores employed in NIST research are activated following a reversible ring-opening mechanism of spirolactam-containing mechanophores. Although mechanophores such as spiropyrans, rotaxanes, and rhodamine 110 spirolactam have been utilized to aid in the characterization of polymer composites, a correlation between mechanophore activation and localized mechanical energy has not yet been achieved.

During the course of the summer, two new mechanophores were synthesized and characterized. These mechanophores were designed based on Jeffamine (increased strain) and 3-aminobenzylamine (delocalization of electron density). Ultrasound mechanical energy was used to determine activation frequencies for mechanophores embedded in an epoxy thermoset matrix. These frequencies were further compared to calculated bond strengths determined by density functional theory simulations.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Grace K Henry | **Award Number**
Academic Institution: University of Maryland | **Major:** Biochemistry

Academic Standing (Sept. '18): First year Ph.D. student (Fall 2018)

Future Plans (School/Career): Complete my Ph.D. in Biochemistry with a concentration in drug development/evaluation and to begin a career in this field.

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Biomolecular Measurement Division, Structure and Function Group [Institute for Bioscience & Biotechnology]

NIST Research Advisor: Prasad Reddy

Title of Talk: Purification of Chorismate Mutase from *M. tuberculosis* for Novel Inhibitor Evaluation

Abstract:

Drug resistant infections, including tuberculosis, pose a huge threat to the global population. There has been a race to identify novel targets in *Mycobacterium tuberculosis* and develop antibiotics that the bacterium cannot develop resistance to. Targeting pathways essential to bacterial life is of great interest. In our study, we targeted Chorismate Mutase (CM) for the identification of novel, small molecule inhibitors. CM plays a central role in the shikimate pathway which is essential for the biosynthesis of the aromatic amino acids; phenylalanine, tyrosine, and tryptophan. This pathway is only present in microorganisms and plants and therefore, as a target, poses little to no threat to humans. The *M. tuberculosis* H37Rv genome has two genes, Rv1885c and Rv0948c, that are responsible for the CM activity. Both code for monofunctional enzymes. Rv1885c contains a N-terminal signal sequence that directs the CM to be secreted from the cell. The Rv1885c gene product is believed to have some chemotactic role in pathogenesis but is also responsible for the majority of the CM activity. The Rv0948c gene product lacks this signal sequence and the enzyme remains in the cytoplasm where the shikimate pathway commonly takes place. In the present study, we exclusively used the Rv1885c gene product. The full-length CM, harboring the signal sequence, was expressed and purified from the periplasmic fluid. In addition, we have completed an activity assay with the periplasmic-isolated CM and inhibition studies are underway. Currently, we are working to express and purify the Rv1885c gene product without the signal sequence, which remains in the cytoplasm. This CM will also be used in activity and inhibition studies. The identification of small-molecule inhibitors for the CM target will be significant in the control and hopefully eradication of drug resistant tuberculosis and other infections.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Allison Horenberg		**Award Number**	70NANB18H129
Academic Institution: University of Virginia		**Major:** Biomedical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Attending graduate school resulting in a PhD in Biomedical Engineering		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Biosystems and Biomaterials Division, Biomaterials Group		
NIST Research Advisor:	Carl Simon, Diane Bienek		
Title of Talk:	Cell Viability in Tissue Engineering Scaffolds		

Abstract:
BACKGROUND: The inability to reliably measure cell viability in engineered tissues remains a major roadblock to the regenerative medicine and tissue engineering industries. Cell viability is a commonly measured product attribute for therapeutic devices that contain cells. Cell viability assays were designed for use in flat culture systems, where the diffusion of assay components is not impeded by the scaffold structure. OBJECTIVE: Assess the ability of an ATP assay system to reliably measure cellular ATP during cell culture in a VitroGel hydrogel scaffold. VitroGel can be disassembled by shear thinning, which enables cells to be released and assayed in the absence of scaffold in order to confirm results conducted on cells in scaffolds. METHODS: The feasibility of measuring cellular ATP in VitroGel hydrogels was assessed. Various aspects of the hydrogel system and ATP assay system were varied to assess their impact on assay response. RESULTS: The VitroGel hydrogel system yielded firm gels as described by the manufacturer. The hydrogels maintain cells in overnight culture and are easily disassembled. The composition of the medium used for the standard curve has a large influence on assay results. When run on gels spiked with ATP, the results were lower than controls without VitroGel. However, a 30 min pre-incubation step allows the diffusion of the assay components to reach an equilibrium so that the results were similar to the controls without gels. When gels spiked with ATP were disassembled by shear thinning, the ATP recovery was 100% as compared to controls without gel. Current work is focused on measuring cellular ATP following gel disassembly by shear thinning. CONCLUSION: The VitroGel and ATP assay are a reliable system for assessing measurements of cell viability in scaffolds.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Eli Janzen		**Award Number**	70NANB18H031
Academic Institution: Kansas State University		**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Graduate Student at Kansas State University		
Future Plans (School/Career):	Graduate School at Kansas State University – Chemical Engineering		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory – Materials Science and Engineering Division – Thermodynamics and Kinetics Group		
NIST Research Advisor:	Ursula Kattner		
Title of Talk:	Calphad Assessments of the Co-Re-Ta and Mo-Ti Systems and Practical Application to the Optimization of hBN Crystal Growth		

Abstract:
The Calphad (shorthand for CALculation of PHAse Diagrams) method is a way to predict thermodynamic quantities and calculate phase diagrams of a given system using semi-empirical models of the Gibbs energy of each phase. Much work is done by researchers in the field to fit the model parameters to available experimental and first-principles data in binary and ternary systems. Once this is done, the assessments of binary and ternary systems may be extrapolated to higher-order, multicomponent systems with good accuracy. This provides a way to reliably predict how a multicomponent system will behave at any given equilibrium condition, greatly reducing the need to experimentally test that system and significantly accelerating materials research.

In this work, assessments were performed on the Co-Re-Ta and Mo-Ti systems as part of work on a larger Co-superalloy database. Other unrelated work focused on the application of existing Calphad assessments to predict the behavior of the B-N-Ni-Cr and B-N-Fe-Cr systems as part of a larger project to grow single crystals of hexagonal boron-nitride (hBN), a valuable semiconductor material. Several key insights have been provided by this research, including that the overall concentration of boron must be kept below 5 wt% to avoid the formation of chromium-borides, that the temperature should be increased from 1550°C to 1600°C to ensure complete melting before crystal growth, and that iron could be used in place of nickel to reduce cost and carbon impurities.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Sally Jiao		**Award Number**	70NANB18H032
Academic Institution: Princeton University		**Major:** Chemical & Biological Engineering	
Academic Standing (Sept. '18):	Graduate Student at the University of California, Santa Barbara		
Future Plans (School/Career):	PhD in Chemical Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Research Group		
NIST Research Advisor:	Harold W. Hatch, Nathan A. Mahynski		
Title of Talk:	Determining Protein and Polymer Stability through Thermodynamic Extrapolation and Active Learning		

Abstract:
Determining the effect of temperature and pressure on biopolymer stability is essential for a variety of applications, such as predicting under what conditions a protein will denature. However, obtaining these trends through molecular simulations is hampered by computational constraints, as atomistic simulations of protein folding can necessitate months of computer time.

Hence, there exists a pressing need to enhance the efficiency of computational methods used to probe these trends. Mahynski et al. demonstrated that data collected from simulations at one thermodynamic state point can be used to predict thermodynamic and structural properties at a different thermodynamic state point, therefore increasing the amount of data that can be extracted from a single simulation. Dai et al., on the other hand, demonstrated that Gaussian process regression and active learning can be applied to intelligently choose thermodynamic state points to sample in the determination of a phase diagram, thus also reducing the number of simulations that need to be performed. Here, we show how those methods can be combined to yield even greater increases in efficiency.

We first demonstrate the utility of thermodynamic extrapolation by generating the temperature-pressure stability diagram of trp-cage, a mini-protein, using the fluctuations to fit a two-state thermodynamic model. We then show how Gaussian process regression and active learning with a simple exploration policy can be applied to efficiently probe the folding of a simple, 5-bead homopolymer. Finally, we incorporate thermodynamic extrapolation into the active learning algorithm and apply the combined technique to the 5-bead homopolymer, comparing the computational cost to that of using either method alone.

We conclude that combining thermodynamic extrapolation and active learning can significantly reduce the cost of probing polymer and protein stability relative to either approach alone.

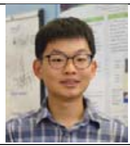
SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: William Jones		**Award Number**	70NANB18H134
Academic Institution: The University of Georgia		**Major:** Genetics	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursue an M.D. / Ph.D Program in Orthopedics		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group		
NIST Research Advisor:	Gil Kaufman		
Title of Talk:	Assessments and quantification of mineralization in dental pulp microtissues by phase imaging		

Abstract:
Untreated dental pulp diseases lead to a root canal procedure which involves the removal of the tissue and leaves the tooth vulnerable to environmental threats. A potential avenue for preserving the dental pulp is to incite cells to differentiate, secrete and deposit dentin mineral, and develop a barrier to protect the pulp from infections. Our goals were: (i) to establish a rapid and efficient dental pulp screening system for inducing mineralization and (ii) to use the system for screening potential materials. 3D dental pulp extracellular matrix (ECM) platform templates composed of immortalized and primary human dental pulp cells were designed for mimicking the biochemical and physiological conditions of the pulp. The mineralization process in the 3D cultures was determined by the deposition and expansion of mineral crystals in the matrix and compared to mineral aggregates (nodules) in the 2D cultures. The deposited mineral levels were validated through phase-contrast imaging analysis. Mineral deposition was tested at 7, 14, and 21 days. Alkaline phosphatase (ALP) assay and Alizarin Red staining was used to track cell differentiation and the progression of mineral deposition, respectively. Quantitative Phase Imaging (QPI) was used to quantify the mineral mass and spread. A µ-Dish 35 mm (micro-dish) was found to improve several parameters of the screening procedure: it lowered the amount of tested materials, reduced the time required to detect mineralization, and kept a stable concentration and volume of the tested component. Mineral deposition was detected in both cell types and became more prominent at progressive time points. Beta-glycerophosphate (BGP) seemed to reach the same mineralization levels as the activation medium; other components such as Tideglusib (TG), fatty-acid derivatives and calcium-phosphate particles (CPC) were also tested. The advanced micro-dish screening platform allows for testing mineralizing agents simultaneously and more efficiently for future use in clinics. BGP was found to be a promising inductive component. The ability to screen for efficient mineralizing materials may help maintain pulp vitality and prevent tissue deterioration and extraction.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Nathaniel Kaneshige		**Award Number**	70NANB18H035
Academic Institution: University of Hawaiʻi at Mānoa		**Major:** Physics and Math	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a PhD in Physics with a focus in particle detection and measurement		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory (MML), Chemical Sciences Division (646), Chemical Process and Nuclear Measurements Group (05)		
NIST Research Advisor:	Dr. Heather Chen-Mayer		
Title of Talk:	Simulation of prompt gamma emission tomography by Compton scattering and the implementation of a neutron tomography system		

Abstract:
At the NIST Center for Neutron Research (NCNR), neutron capture induced Prompt Gamma Activation Analysis (PGAA) has long been applied as a method for nondestructively studying bulk sample compositions. MML is currently developing a 3D tomographic imaging system to expand the PGAA technique for obtaining structural information and material distribution within a sample through the novel application of Compton Imaging and Neutron Tomography systems. Building on previous work, we expand the functionality of a Geant4 detector simulation of the gamma ray emissions and the CdZnTe detector system and perform tomographic reconstruction by back projection of the Compton cones. We study how detector parameters, gamma ray source geometry, and gamma ray spectral characteristics affect the spatial resolution for the system given the number of incident events. Experimentally, in collaboration with PML, a neutron tomography system was also implemented for obtaining complementary structural information for a given sample. These results will be applied to the continuing development of a 3D imaging system for expanding the PGAA capabilities at the NCNR.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Kamryn Kant		**Award Number**	70NANB18H141
Academic Institution: Clemson University		**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Graduate Student at Clemson University		
Future Plans (School/Career):	Pursuing a PhD in Chemical Engineering at Clemson University		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Research Group		
NIST Research Advisor:	Dr. Nathan Mahynski		
Title of Talk:	Computing Thermodynamic Properties of Fluids Confined in Nanoporous Materials with High-throughput Molecular Simulations		

Abstract:
Multicomponent fluid adsorption into nano- and mesoporous adsorbents is a complex process which can be difficult to model at a molecular level. New and improved theories are required to describe an ever-increasing amount of complex adsorbent and adsorbates under a broad range of conditions; however, theory development requires a large amount of data. While straightforward computer simulation techniques can be employed to generate this data, the computational expense can be prohibitive. Recently, an alternative technique has been developed that allows for the accurate extrapolation from data generated by flat-histogram Monte Carlo simulations. This method greatly increases the amount of information gained from simulations while maintaining a high degree of accuracy, and therefore reduces the computational expense. This extrapolation method was utilized to generate adsorption isotherms of binary fluids confined in nanopores in equilibrium with a bulk fluid. Monte Carlo simulations in the grand canonical ensemble were performed on the bulk and confined systems separately, wherein the chemical potentials of species 1 ($\mu 1$) and species 2 ($\mu 2$), volume, and temperature were fixed while the number of particles and pressure were allowed to fluctuate.

We investigated how a bulk fluid at a certain mole fraction will behave when placed in a range of different characteristic adsorbents. To do this, we computed isopleths, or parametric paths of chemical potentials at a constant mole fraction, for each bulk fluid at various temperatures. These chemical potential values were used to calculate the properties of the confined system which is in equilibrium in with the bulk phase. Adsorption isotherms and selectivity curves were generated from these confined and bulk properties. Eventually, isotherms for eight representative binary mixtures and 108 porous materials at 13 different temperatures will be calculated and stored in an open-source database, which will allow researchers to develop and test new theories related to adsorption.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Klara Keim		**Award Number**	70NANB18H142
Academic Institution: Texas Tech University		**Major:** Microbiology	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing an M.D./Ph.D Program for later work in Infectious Diseases.		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group.		
NIST Research Advisor:	Stella Alimperti		
Title of Talk:	Development of Microfluidic Platforms Recapitulating Oral Microvasculature		

Abstract:
Oral microvascular diseases are strongly correlated to other diseases, such as oral cancer, diabetes, and hyperglycemia-induced periodontitis. Buildup of plaque around veins, arteries, and microvessels alters blood vessel morphology by restricting or altering blood flow. Therefore, the need of proper therapeutic and pharmacological interventions is necessary. However, current in vitro vascular models lack an accurate representation of complex in vivo conditions. Furthermore, in vivo models are expensive, and it is difficult to control many parameters within a single, and often living, model, which leads to time consuming and expensive development of the proper drug treatment. The demand of overcoming these limitations and developing novel therapeutics based on personalized medicine for microvascular diseases is necessary. The current research aims to develop personalized medicine for microvascular diseases and also to develop novel technology based on the organ-on-a-chip technology. This microfluidic device is mimicking human microvasculature, quantifying spatiotemporally changes during microvascular angiogenesis, and measuring the impact of shear stress and fluid flow within the system. The scaffold of this microfluidic devices has been 3D printed and customized using polydimethylsiloxane (PDMS). The human umbilical vein cells (HUVECs) are seeded into a cylindrical collagen matrix and allowed to form a proper 3D vascular structure. The engineered vasculature was then used to mimic physiological responses to shear stress and controlled fluid flow. We have shown the microvessels respond through quantifiable deformation of the channel diameter, specifically expanding in instances of increased pressure and flow followed by contraction. Structural changes in vessel deformations were visualized by changes in cell-cell contact and actin organization using immunostaining techniques. These microfluidic devices allow for the development of dynamic multiparameter systems, enabling generation and quantification of fluid flow, shear stress, and multicellular interaction. Therefore, this technology will provide a high throughput, simple, and accurate predictive model for human microvascular diseases and physiology in addition to efficient experimental drug development in vitro.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Julianna Koehl		**Award Number**	70NANB18H081
Academic Institution: Lebanon Valley College		**Major:** Chemistry	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Attend Graduate School for Chemistry or Polymer Science		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group		
NIST Research Advisor:	Joel M. Sarapas		
Title of Talk:	Optimization of Ring Expansion Cationic Polymerization as a Route to Ideal Networks		

Abstract:
Polymer networks are a universal engineering material, spanning countless fields from biomedical to automotive. Network architecture has been shown to have a profound effect on material properties, though the presence of defects (e.g. dangle chains) can contribute and sometimes overshadow desired attributes. Cyclic polymer networks offer a route to defect-free materials, but are not widely accessible or characterized. In order to improve access to this class of networks, a synthetic route to cyclic polymers that is experimentally feasible, scalable, and functional group tolerant is required. Here, we apply ring expansion cationic polymerization, which fulfills all our above requirements. A cyclic hemiacetal ester was synthesized first and provided a foundation for polymerizing isobutyl vinyl ether. A norbornene functionalized ester was then copolymerized with the isobutyl vinyl ether, giving a mode to crosslink using click chemistry. The copolymerization of the two monomers was successful, as both polymerized at similar rates, giving a uniform material. These polymers by themselves present unique properties to their linear counterparts.
Crosslinking the functionalized copolymer through thiol-ene click chemistry yields networks free of dangling ends. These materials are of particular interest mechanically, and have the potential to be investigated by KESO or fracture using laser-induced projectile impact test (LIPIT). With these mechanics studies, an improved fundamental understanding of polymer networks is gained that can broadly be applied to both academic and industrial materials design.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Alison Kriz		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Materials Science and Engineering	
Academic Standing (Sept. 18):	Junior		
Future Plans (School/Career):	Pursuing a graduate degree in Materials Science and Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Functional Polymers Group		
NIST Research Advisor:	Vladimir Oleshko, Christopher Soles		
Title of Talk:	High-Aspect Ratio Sulfur-MoS_2-Carbon Heterostructure Electrode Materials for High-Performance Li-S Batteries: Design and Multiscale Characterization by Advanced Focused Ion and Electron Beam Techniques		

Abstract:

Emerging applications of electrical energy storage technologies in transportation, portable electronics, and national security rapidly increase the demands for the next generation of rechargeable electrochemical batteries with high energy density and long cycling life. The lithium-sulfur (Li-S) battery is a promising candidate technology because of its high theoretical specific energy and high specific capacity, as well as the low cost, natural abundance, and nontoxicity of elemental sulfur. However, due to the electrochemical conversion of sulfur into lithium polysulfides (Li_2S_x, x = 3-8) during discharge, cathodes experience capacity fading, poor Coulombic efficiency, and limited life cycle, thus limiting the practical realization of Li-S technology.

In this project, we explore the integration of sulfur with graphene and nanocrystalline transition metal dichalcogenides TMX_2 (TM = Mo, W, X = S, Se, Te) to produce heterostructures capable of electrocatalytically converting Li_2S_x (x = 6-8) into insoluble Li_2S, reducing the effective diffusion lengths of the polysulfides, stabilizing 2D sulfur layers, and improving the rate capabilities of the cathodes. We employ a combination of advanced focused ion beam and analytical electron microscopy techniques to investigate the topography, morphology, interfaces, crystallinity, and chemical compositions in the heterostructures at multiple scales up to the atomic level and compare with those for MoS_2-S_8 composite-based cathodes fabricated using the traditional slurry-based scheme.

We used waste-free, low-pressure vapor deposition to fabricate nanostructured sulfur coatings on the surfaces of graphene and TMX_2. We found that graphene flakes coated with sulfur demonstrate thin island-like layers composed of partially coalescing sulfur nanoparticles on the surfaces of wrinkled nanosheets. Casting additionally TMX_2 flakes, we produced sandwich heterostructures involving nanolayers of highly conductive graphene, sulfur, and TMX_2, which potentially enable high surface area robust interfaces with improved electronic and ionic conductivity and charge transfer as well as enhanced physical integrity of the composite cathodes.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Simin Manasiya		**Award Number**	70NANB18H125
Academic Institution: University of Houston		**Major:** Biomedical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory (MML), Materials Science and Engineering Division (MSED), Polymers and Complex Fluids Group		
NIST Research Advisor:	Alexandros Chremos		
Title of Talk:	Polyelectrolyte stiffness in different salt concentrations and salt types		

Abstract:

Polyelectrolytes, like DNA and proteins, play an essential role in carrying out and regulating important cellular functions and they are often encountered in aqueous solvents with varying salt concentrations. In particular, ions that result from salt dissociation in water, influence the conformational properties of the polyelectrolyte chain when they are present in its immediate vicinity. Our focus is on the quantification of the polymer stiffness of a bead-spring polymer model in aqueous solutions at different salt concentrations. Our model explicitly describes four types of molecules: a linear polymer chain, H_2O molecules, counter-ions, and co-ions. Additionally, we examine three different salt types (NaCl, CsI, KBr); since ions influence the cohesiveness of the liquid depending the strength of the ion solvation affinity and by extension, affecting the polymer conformations. Molecular dynamics (MD) simulations were performed with LAMMPS package and Python programs were developed to automate the process generating the initial configurations and analyzing the trajectories generated from MD simulations. We find that in salt-free solutions, the polymer chain swells and becomes stiff due to the electrostatic interactions between the charges along the polyelectrolyte backbone. Upon the addition of salt, the electrostatic interactions are screened, resulting in the polyelectrolyte chain to adopt more flexible and compact configurations. Different ion types can enhance or suppress the effects of screening depending on the strength of ion solvent affinity.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Sabrina Martin		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Bioengineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Complete bachelor's degree and pursue a career in bioengineering.		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Surface and Trace Chemical Analysis Group		
NIST Research Advisor:	Greg Gillen		
Title of Talk:	Drop-On-Demand Inkjet Printing for Preparation of Oral Drug Delivery Films		

Abstract:

Dissolvable oral thin film (OTF) drug delivery films are gaining interest as alternatives to conventional tablets and capsules. OTFs are typically made by mixing an active pharmaceutical ingredient (API) into a dissolvable polymer that is administered by buccal or sublingual routes. Direct adsorption of the API into the systemic circulation bypasses gastrointestinal delivery and provides increased bioavailability and rapid release. OTFs are currently manufactured as sheets with fixed levels of API. This is a roadblock to the use of OTFs for personalized medicine with patient-specific API dosages. One method being explored is drop-on-demand inkjet printing to deposit individualized API doses onto prefabricated films.

In this work we explore inkjet printing onto model OTF films using acetaminophen as the API compound. Areas of focus include; (1) development of standard printing conditions, (2) quantitative measurement of the deposited API dose, (3) API dissolution characteristics and (4), characterization of the chemical form of the printed API. UV-Vis spectroscopy was used to determine the mass of API printed onto model film surfaces. Comparison of UV-Vis spectroscopy and gravimetric based measurements indicate that the concentration calculated from both agree within less than 1% RSD. Acetaminophen was printed onto silane treated silicon wafers in various array configurations at a mass of 0.112 mg/sample. Drug dissolution testing of each array was based on a USP paddle type apparatus, where the printed wafer was submerged in 8 mL water with 60 rpm stirring speed. 500 µL samples were withdrawn for quantitative UV-Vis measurement. API release profiles were found to be influenced by the array characteristics suggesting the ability to tailor drug release characteristics. Inkjet printing was also found to create various API polymorphs which were evaluated with Raman and THz Raman spectroscopy. Current studies are aimed at extension of this work to printing on real OTF film substrates.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Kevin McCright		**Award Number**	70NANB18H153
Academic Institution: University of Maryland College Park		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Attend Graduate school in engineering		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science and Engineering Division, Thermodynamics and Kinetics Division		
NIST Research Advisor:	Sheng Yen Lin		
Title of Talk:	Uncertainty Quantification and Propagation in Carbon Steel Machining		

Abstract:

Machining carbon steels is common place and being able to quantify modeling uncertainties is important in developing low cost, efficient, and safe products. Although carbon steels have been well documented in their behavior, advancements in other areas bring new situations that haven't yet been tested. Using sample data from the Kolsky bar, which tests super heating and high strain rates, I implemented the computational module to quantify the modeling uncertainty and its propagation to calculate the stress-strain curve. This module helps to assess the reliability of the integrated computational materials engineering framework (ICME) in order to create accurate representations of the mechanical properties of carbon steels. The module quantifies the modeling uncertainties of yield stress and strain hardening by using deterministic and probabilistic regressions that would be able to fit the data from experiments and quantify the uncertainties. Using this module in the ICME framework would be able to predict the stress-strain curve under the super heating, high strain rates deformation in the Kolsky bar experiment. These results will be used to create a more advanced machining simulation that would be able to handle more processing conditions for carbon steels.

SURF Student Colloquium

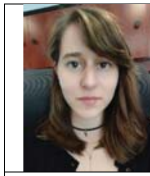
NIST – Gaithersburg, MD

August 7-9, 2018

Name: Hallie Miller		**Award Number**	70NANB18H097
Academic Institution: University of Utah		**Major:** Materials Engineering	
Academic Standing (Sept. '18):	1st year graduate student		
Future Plans (School/Career):	Ph.D. in Materials Science and Engineering		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Microscopy and Microanalysis Research Group		
NIST Research Advisor:	Donald Windover		
Title of Talk:	Illuminating the transparency of glass elemental composition		

Abstract:

This study uses NIST Standard Reference Materials (SRMs) to investigate the utility of Micro X-ray fluorescence (µXRF) to analyze trace elements in bulk materials. SRMs serve two primary purposes: to define benchmarks for composition and quality of various materials and to test the calibration and sensitivity of measurement methods using SRMs as independent reference standards. µXRF Spectroscopy is an elemental analysis technique that identifies elements by their characteristic x-ray emissions. This technique uses a focused x-ray source to illuminate and fluoresce a small lateral area of a sample, thus allowing for detailed analysis and mapping of the elemental composition on a micrometer scale. SRM 610 and 612 are homogeneous composition glasses which are primarily made up of a SiO_2, CaO, Na_2O and Al_2O_3 bulk matrix with over 40 additional trace elements. Through taking a wide array of measurement points of the SRM 610 and 612 glasses under various beam conditions, this study aimed to accurately compare the measured mass percentage of each glasses elemental composition to their documented values. Two different software packages were used to distinguish data fitting methodologies and to compare how each software package handles composition analysis. Results show that preliminary quantitative results are hindered by background subtraction routines, separation of K,L,M shell element line overlaps, and improperly implemented instrument calibration models. This technique excelled at identifying qualitatively the presence of trace elements, however due to the discovered constraints of µXRF, quantitative results are still limited by the analysis tools available which provides an area for future research.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Elena Musteata		**Award Number**	70NANB18H110
Academic Institution: SUNY PI Colleges of Nanoscale Science and Engineering (CNSE)		**Major:** Nanobioscience & Applied Mathematics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	In my graduate studies, I hope to conduct research in bioengineering, specializing in genetics as applied to drug development and delivery.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biosystems and Biomaterials Division, Complex Microbial Systems Group: Engineering Biology Team		
NIST Research Advisor:	Dr. David Ross		
Title of Talk:	Synthetic Biology for Living Sensors: Characterizing Fitness Landscapes of Engineered Genetic Circuits		

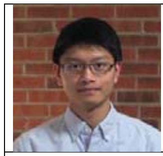
Abstract:

Synthetic biology is a relatively new field based on the idea that it is possible to genetically reprogram the inner workings of cells and thereby change the way they sense and respond to their environments. It offers promising solutions to some of our most pervasive pharmaceutical, agricultural, and energy-related problems. The key elements in this cellular reprogramming are genetic sensors, which are typically proteins that regulate cellular gene expression based on external stimuli. Developing a means to engineer new, metabolically efficient genetic sensors with high specificity, sensitivity, and tunable performance standards is prerequisite to sensor implementation within living therapeutics or industrially-applicable manufacturing platforms. Critical limitations must be overcome before the field can advance and realize its revolutionary potential. In particular, no methods currently exist for predictive engineering of genetic sensors, and thus no robust foundation upon which to design novel organisms capable of sensing and reproducibly responding to specific input signals within dynamic environmental conditions.

The Engineering Biology team at NIST aims to address these limitations by creating a hybrid bio-machine learning platform that will allow for the engineering of living sensors in a predictive, scalable, and quantitative way. A first-phase objective of this project is to develop optimization algorithms capable of using measurements of complex biological fitness landscapes to identify the DNA sequences that encode genetic sensors with the desired characteristics. To measure these fitness landscapes, we have started by designing a DNA construct that serves as a selection mechanism by tying cell survival to sensor performance, allowing us to exploit natural evolutionary pressures to evolve optimized sensors for customized response curves.

Our first working genetic circuit is based on the native bacterial system for sensing the sugar lactose and has two functional components, the regulatory sensor and a set of actuator genes. We are building a library of sensor variants by introducing random mutations into the sensor elements of the circuit, some of which will alter the response curve and binding affinity to the molecule being sensed. The fitness of these mutants will be assessed using multiple metrics and across a variety of conditions, providing an abundance of data for training our AI. To run these experiments with an adequately high-throughput approach, we are creating a novel combinatorial process flow that integrates next-generation sequencing and library construction techniques.

The resultant algorithms will facilitate the efficient and predictable programming of sensor systems to respond to non-native molecular substrates, with prescribed input-output curves capable of matching environmental fluctuations. This offers a generalizable process to design sensors for any input signal. Sensors like these can then be combined to produce living measurement systems that take advantage of the cell's own machinery to produce products and perform useful functions for applications ranging from personalized medicine to environmental remediation.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Daniel Ng		**Award Number**	70NANB18H075
Academic Institution: Northwestern University		**Major:** Materials Science and Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Attend graduate school for PhD in materials science		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Mechanical Performance Group		
NIST Research Advisor:	Mark Stoudt		
Title of Talk:	Optimizing Additively Manufactured Inconel 625 for Reliable Performance		

Abstract:

Additive manufacturing (AM) is a rapidly developing technology with promising industrial applications for fabrication of parts with complex geometries, and an increasing number of metal alloys are being considered for use in the AM process. One such material is Inconel 625 (IN625), a nickel-based superalloy widely used in marine, nuclear, and aerospace applications due to its mechanical stability at high temperatures, as well as corrosion and oxidation resistance. However, the AM process generates microstructures that are significantly different from the ones observed in traditional wrought form, raising the possibility of unexpected or unreliable performance. This project is part of an ongoing effort to examine how microstructural evolution during AM processing and post-build heat treatments affects the mechanical properties, corrosion resistance, and resistance to environmentally-induced cracking mechanisms such as stress corrosion cracking (SCC) or hydrogen embrittlement (HE).

A combination of scanning electron microscopy, electron backscatter diffraction, and energy dispersive spectroscopy were used to characterize the microstructures of wrought IN625 and heat-treated AM samples. The electrochemical performance of samples was assessed with two techniques: a linear polarization resistance measurement for the corrosion rate, and a potentiodynamic polarization measurement for the resistance to localized attack (pitting). Both measurements were conducted in 0.1 M HCl.

Results from the electrochemical measurements provide a framework for conducting slow strain rate tensile tests (SSRT) that will evaluate the susceptibility to environmentally-induced cracking. These evaluations will help determine whether the mechanical and electrochemical performance of AM IN625 are consistent with those of the wrought material. The ultimate goal of this work is to establish whether the existing performance models developed for wrought IN625 may be applied to the AM material.

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August 7-9, 2018

Name: Charlie Nitschelm		**Award Number**	70NANB18H077
Academic Institution: University of New Hampshire		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Attend a graduate school for aerospace engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory - Materials Science and Engineering Division Mechanical Performance Group		
NIST Research Advisor:	Steven Mates		
Title of Talk:	Mechanical Measurements of Inconel 625 for Dynamic Forming Simulations		

Abstract:

This project focuses on the mechanical behavior of Inconel 625 (IN625) at various temperatures and strain rates to better understand how the material behaves during dynamic metal forming processes. IN625 is a desirable material in many areas of industry for its high temperature strength, corrosion resistance, and its good formability and weldability. In dynamic metal forming processes, the material will be subject to high strain rates and temperatures so it is important to characterize its behavior under these extreme conditions. Specifically, the degradation of mechanical properties near 700 °C may involve the gradual growth of brittle carbides or precipitates, which introduces the possibility that the strength of IN625 is time-dependent under dynamic forming conditions, where heating times are short and strain rates are high. To probe this possibility, I use a specialized pulse-heated Kolsky bar to measure the mechanical response at high strain rates in tension and compression and under rapid heating in compression up to 1000 °C. In addition, I use a servo-hydraulic test frame to measure the low strain rate response in tension up to fracture. These data are used to calibrate the Johnson-Cook flow stress model, which can accurately capture strain hardening, strain-rate hardening and thermal softening in many metal alloys. The calibrated model will then be used to simulate the dynamic forming of laminate components for a heat exchanger to allow electricity to be created from high temperature waste heat from industrial exhaust which currently adds up to 2.4 million kWh (or 8,000,000,000 gallons of gasoline)

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Rachel Orenstein		**Award Number**	70NANB18H075
Academic Institution:	Northwestern University	**Major:** Materials Science and Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursue a career in industry and an advanced degree		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group		
NIST Research Advisor:	Zachary Trautt		
Title of Talk:	Building a resource registry and data repository for High-Throughput (Combinatorial) Experimental materials research		

Abstract:
Researchers are increasingly recognizing the need for improved management of scientific data. With so many different sources and caches of information, it can be challenging to find the right data, and even when identified, it can be almost impossible to extract for use in other formats. The Materials Genome Initiative and the FAIR data principles were consequently established to address this issue and set the framework for a more organized future. The Materials Genome Initiative was launched in 2011 to accelerate the development of advanced materials and focuses significantly on making digital data accessible. The FAIR principles call for data to be Findable – containing metadata that uniquely describes the contents of the dataset and searchable; Accessible – accessed using a universally applicable, standard method; Interoperable – easily translatable from one format to another; and Reusable – understandable to multiple informed parties.

To help answer the call for a better data management system, the Configurable Data Curation System (CDCS) was developed at NIST. The CDCS is a customizable application which allows users to format data into an XML structure using XML Schema. The High Throughput Experiment (HTE) Repository is a customized instance of the CDCS used to store and display materials measurement data from high throughput experiments including x-ray diffraction and spectroscopy. While this service is currently optimized for machine-actionable data, improvements were needed to improve human interaction with deposited data. Throughout the course of the summer, I developed online data visualization tools using technology such as the JavaScript D3.js library and XSL. Additionally, I created templates to export the data into usable formats such as text files and comma separated value files. The implementation of these tools will greatly improve the user experience of the repository.

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Name: Patrick Ott		**Award Number**	70NANB18H153
Academic Institution:	University of Maryland College Park	**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursue a graduate degree in chemical engineering and a career emphasizing sustainability		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory; Division 643; Security Technologies Group		
NIST Research Advisor:	Qi An; Aaron Forster		
Title of Talk:	Structure-property relationships in multi-functional hierarchical fiber nanocomposites		

Abstract:
Fiber reinforced polymer (FRP) composites have been used extensively in the automotive and aerospace industries due to their high strength to weight ratio. Recently, the incorporation of conductive nanofillers, such as carbon nanotubes (CNTs), into FRP composites creates multifunctional materials with improved mechanical properties and capabilities for damage monitoring. The primary method to manufacture these complex FRP composites is by direct grafting of CNTs to the surface of the microscale reinforcing fibers. This is a challenge because chemical vapor deposition involves high temperatures that are detrimental to fiber adhesion promoters (sizing) and may damage the fiber strength by introducing flaws. A process that is friendlier to current FRP materials is electrophoretic deposition (EPD). This is an industrial coating process in which a charged CNT solution complex is directly deposited onto the microscale fiber preform using an electric field. This allows for low-energy production of thicker, more homogenous CNT films onto fiber surfaces in a controlled fashion. While this process has been successfully used to create multifunctional composites, there is no quantitative protocol to evaluate the EPD process. This project examines the efficacy of functionalization and deposition of CNTs onto glass slides and gold coated silicon surfaces, a 2D simplification for the fiber geometry. The deposition rate, and thus viability, of functionalization was analyzed by identifying changes in the carbon-oxygen ratio over time with energy-dispersive X-ray spectroscopy (EDS). Additionally, the effect of film forming additives, polyethyleneimine (PEI), on the thickness and uniformity of the CNT film onto the surfaces is examined with scanning electron microscopy (SEM). Finally, differential scanning calorimetry (DSC) is used to evaluate the effect of the CNT layer on the curing process of relevant epoxy-amine FRP matrix materials. The impact of CNT functionalization and deposition parameters on composite mechanical and electrical properties is also discussed.

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August 7-9, 2018

Name: James Riet		**Award Number**	70NANB18H109
Academic Institution:	Virginia Polytechnic Institute and State University	**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Attending graduate school in pursuit of a PhD in Chemistry		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science Division, Surface Trace Chemical Analysis Group 643.05		
NIST Research Advisor:	Shin Muramoto		
Title of Talk:	An Evaluation of Polymer Encapsulation as a Means of Minimizing the Degradation of TNT for Explosive Trace Detectors		

Abstract:
Encapsulation, often used in the food and pharmaceutical industries, involves the incorporation of a molecule, cell, enzyme or any other desired substance in an encapsulant, which resists undesired moisture, heat, or other conditions which may not be conducive to the stability of the substance. In this proof of concept study, we are interested in monitoring the stability of the explosives with and without encapsulants and proving encapsulation to be a simple, safe, and effective measure to prevent degradation of test materials that are later used for our involvement with the calibration and verification of Explosive Trace Detectors (ETD). Test materials that contain trinitrotoluene (TNT) are subject to compositional degradation due to certain environmental conditions, and polymer encapsulation is thought to prevent degradation over the periods of time that are specifically seen in these studies. Two encapsulants, polyvinylpyrrolidone (PVP) and polymethylmethacrylate (PMMA) were considered in the study. The encapsulated TNT was printed onto test materials and was then analyzed on the ion mobility spectrometer (IMS) time-of-flight secondary ion mass spectrometer (ToF-SIMS). During a temporal study conducted over a period of 50 days, encapsulation at concentration of .1% and .5% polymer generally seemed to prevent degradation. On one IMS, detectability of TNT remained strong and unchanged duration of the study regardless of encapsulation, suggesting that there is no degradation encountered over the time period. Thereby, even at .1% concentration, these polymers are effective encapsulants against the degradation of TNT as the TNT remains more detectable for longer periods of time. In all cases the TNT only remains more detectable for longer periods of time when it is encapsulated. Encapsulation has seemed to serve its intended purpose as a safe, easy-to-implement, and effective measure against TNT degradation.

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August 7-9, 2018

Name: Viviana Rodriguez C.		**Award Number**	70NANB18H099
Academic Institution: Montgomery College		**Major:** Bioengineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing a bachelor's degree in Bioengineering from the University of Maryland College Park, and a future master's degree in science policy.		
NIST Laboratory, Division, and Group:	MML, 642		
NIST Research Advisor:	Dr. Sara Orski		
Title of Talk:	Method Development and Depth-Profiling Degradation Measurements of Beach Plastics.		

Abstract:
Every year, an estimated 8 million metric tons of plastics get into the world's oceans and beaches causing significant damage to the marine ecosystem. Pelagic animals are at high risk of getting entangled in plastic nets or confusing plastics for food, frequently with catastrophic consequences such as asphyxiation or dead by starvation. In order to understand the extent of potential damage that plastics can cause in the marine environment, it is necessary to study how these synthetic polymers degrade in such environmental conditions. In the marine ecosystem, plastics are initially exposed to abiotic degradation in the form of photo-oxidation by UV light radiation, thermodegradation, and hydrolysis. Once the polymer's carbon backbone has been sufficiently degraded through termination of a free radical reaction that leads to chain scission, smaller polymer chains are available to be degraded by microorganisms in what is known as biodegradation. The purpose of this research study is to develop an accurate method to measure polymer degradation as a function of depth in beach plastic samples. Initially, 63 plastic pieces collected at Kaupo beach, Hawaii, were categorized based on their thickness. From this total, 48 samples were selected as optimal for identification and characterization by X-ray photoelectron spectroscopy (XPS). As a result, 31 of these plastics were found to be polyethylene (PE), 11 polypropylene (PP), 1 PE/PP mixture, 1 polyethylene terephthalate (PETE), and 4 unknown. Considering that PP offers a more interesting degradation pathway due to its lower stability compared to PE, and its higher susceptibility to abiotic degradation, PP was selected for depth profiling degradation studies by XPS, high temperature gel permeation chromatography (GPC), and differential scanning calorimetry (DSC). These techniques have shown a clear decrease in the average molar mass distribution, a high degree of oxidation, and greater incidence of foreign chemical elements at the exposed surface relative to the deeper material core. Ultimately, this research can be used to aid the marine scientific community for sampling plastic marine debris, by providing them with alternate techniques of identification, and degradation measurements, that can eventually translate into conservation efforts, and a cleaner and safer ocean for all.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Emily Roe		**Award Number**	70NANB18H083
Academic Institution:	North Carolina State University	**Major:** Materials Science and Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Graduate studies in Materials Science		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science and Engineering Division, Polymers Processing Group		
NIST Research Advisor:	Lee Richter, Ahmad Kirmani		
Title of Talk:	Blade-coating as a scalable route to metal oxide field-effect transistor fabrication		

Abstract:
Metal oxide field effect transistors (MOFETs) have wide-ranging applications in the electronics industry are a promising cost-effective alternative to silicon for large area applications such as displays. To date, MOFETs have usually been fabricated using vapor deposition, a subtractive process requiring high annealing temperatures and removal of oxide. Considerable interest exists in solution-based processing, which requires lower annealing temperatures, is compatible with flexible substrates, and supports additive, print-based patterning. The most common solution-based deposition process is spin-coating, which cannot easily scale to large area deposition. This project explores blade-coating as a viable, scalable route to fabricating Indium Oxide (In2O3) FETs.

Two metal oxide solutions were characterized, a simple sol-gel and a combustion enhanced solution. Following optimization of In2O3 blade coating conditions, each solution was used to make In2O3 thin films (~20 nm) in bottom-gate top contact field-effect transistors. FET fabrication entailed blade coating the solutions on pre-cleaned 230 nm SiO2/Si substrates followed by thermal annealing in the 200 to 300 □C range. Subsequently, 70 nm Al source and drain electrodes were thermally deposited. Saturation electron mobilities (µsat) of ~4.5 cm^2/Vs were obtained for the sol-gel recipe, albeit with large negative threshold voltages (Vth), similar to current reports on spin-coated devices. Notably, the optimized anneal temperature for bladed sol-gel FETs was significantly lower than the reported optimum temperature for the spin-coated counterparts. The combustion enhanced solution required higher anneal temperatures than the sol-gel solution. To address the high Vth, likely due to oxygen vacancies in the metal oxide lattices, ultraviolet (UV)-ozone treatment and solution chemical modifiers were investigated.

Initial results indicate an improvement in Vth with UV-ozone treatment. These findings establish blade-coating as a viable route to scalable fabrication of In2O3 FETs a step forward in making In2O3 FETs viable for the electronics industry.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Sejal Shah		**Award Number**	70NANB18H118
Academic Institution:	University of Delaware	**Major:** Biomedical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Attend graduate school for biomedical engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science Division, Security Technologies Group		
NIST Research Advisor:	Ran Tao		
Title of Talk:	Rheology of shear thickening fluids		

Abstract:

Shear thickening fluids (STFs) are non-Newtonian fluids that reversibly, transition from a liquid to a solid phase at high levels of stress or high strain rates. Shear thickening behavior is commonly observed in concentrated suspensions composed of solid particles in a liquid medium. At a critical stress or strain rate, the repulsive forces between the suspended particles are overcome and the particles form solid structures, called hydroclusters. The clusters quickly aggregate in the flow field which increases the solution viscosity and absorbs energy. The hydroclusters will separate after stress is relieved and the substance reverts to a liquid state. STFs have promising applications as energy absorbing additives in protective clothing and sporting equipment. While there are some benefits, STFs also have the potential to cause detrimental effects in industrial settings such as blocking fluid flow in pipes. A recent study shows that an orthogonal superimposed perturbation (OSP) to the primary shearing flow, may strategically control shear thickening behavior. OSP has the potential to significantly lower the viscosity of the suspension by introducing a disturbance large enough to cause the hydroclusters to disassemble which allows the material to flow like a liquid. In this study, we perform steady shear and oscillatory shear measurements on cornstarch and water mixture and glass spheres and glycerol suspensions STF systems. These measurements define the critical stress and strain rate for STF response. We utilize the OSP technique to introduce biaxial shear to the STFs, in hopes of obtaining tunable shear thickening behavior as well as a fundamental understanding of this behavior.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Ryan Smith		**Award Number**	70NANB18H125
Academic Institution:	University of Houston	**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue PhD		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group		
NIST Research Advisor:	Jason R. Hattrick-Simpers		
Title of Talk:	Predicting the Elastic Properties of Metallic Glasses with Machine Learning		

Abstract:
Metallic glasses (MG), also known as amorphous metals, are highly sought-after materials due to their exceptional physical and chemical properties, such as high toughness and corrosion resistance. These properties make them desirable for applications such as bone implants, high efficiency transformers, and electrical contacts. However, their stability and properties are not readily predicted by standard physicochemical theories or empirical heuristics. With an appropriate material representation, machine learning accurately predicts MG stability. This study focuses on extending this approach to determine ML models which accurately predict material properties. A literature survey was conducted to compile a starting data set for training the models. This study used MAGPIE, the Materials-Agnostic Platform for Informatics and Exploration, to generate composition-based attributes used to train predictive ML models. ML tools and algorithms from Weka (Waikato Environment for Knowledge Analysis) and the Python library scikit-learn facilitated the development of data-driven models. We tested many types of regression models, including random forest, Gaussian processes, and support vector machines, and evaluated their predictive accuracy for the elastic properties of MG. We found that random forest regression models were consistently the most accurate, with the highest values for the coefficient of determination for 10-fold cross-validation out of all models tested. In addition to directly increasing the accuracy of elastic property predictions, the models created in this study will enable a "jump start" to an adaptive design of experiments. Such experiments will intelligently guide sparse data collection, maximizing knowledge gained per data point. Elastic property measurements are slow, so reducing the number of necessary experimental measurements will significantly reduce the time and resource cost of developing new metallic glasses.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Nicholas Strogen		**Award Number**	70NANB18H064
Academic Institution:	West Virginia University	**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate studies in Materials Science and Engineering		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Sience and Engineering , Functional Polymers Group		
NIST Research Advisor:	Velencia Witherspoon, Christopher Stafford		
Title of Talk:	The Effects of Chlorine Exposure on the Performance and Morphollogy of Polyamide Membranes		

Abstract:
Reverse osmosis (RO) membranes are responsible for 80% of the world's water desalination plant. Commercial membranes are typically composed of a thin (~100 nm) polyamide (PA) active layer and porous mechanical support which have been empirically developed by industry for the high fluxes of water and high salt rejection of common ions found in seawater (i.e. NaCl). After numerous desalinations, the membranes often suffer a loss in this performance from biofouling, treated by chlorine based disinfected agent that is known to cause degradation to active layer affecting its durability and reliability over many cycles. Previous work has correlated chlorine exposure with structural changes indicated that defect by bond breaking may be introducing defects in the PA. Despite the common use of these membranes, little is known about the chlorination effects the polyamide bonds and the ability of membrane to resist salt resistivity transport across the membrane.

The performance of 5 industrially manufactured membranes was characterized by both macroscopic and microscopic techniques in terms of permeability and chemical structure. Electrical Impedance Spectroscopy methods were developed in addition to common salt rejection measurements to track the resistance to NaCl transport before and after chlorination. Scanning Electron Microscopy (SEM) allowed us to obtain data about the polyamide pore structure. While solid-state nuclear magnetic resonance, a robust method commonly used to quantify the chemical bonds in polymer materials, was used to gain insight to the chemical changes due to chlorination and correlated with membrane performance.

Results produced in the final weeks will be discussed in this presentation.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Claire Liliane Sturek		**Award Number**	70NANB18H095
Academic Institution: The Catholic University of America		**Major:** Biomedical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing medical school after graduation, with plans to achieve both a M.D. and Ph.D.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biosystems and Biomaterials Division, ADA Foundation-Volpe Research Center (644, 03)		
NIST Research Advisor:	Diane Bienek Ph.D., Drago Skrtic Ph.D., Nancy Lin Ph.D.		
Title of Talk:	Antimicrobial Properties of Novel Class V Restoratives		

Abstract:
Dental caries are among the most common medical conditions reported in the United States. They occur when sticky bacterial communities on tooth surfaces, called plaque, erode enamel via their acidic metabolic byproducts. This deterioration becomes more serious when plaque extends below the gum line or into periodontal pockets that are not easily cleaned from brushing or saliva, rendering the root surface more susceptible to corrosion. Resin-based dental composite materials are used to repair root decay in what is called a Class V restoration. However, due to the sheltered nature of the location, secondary caries often occur and remain the dominating reason for failure (≤ 9.43% annual) of existing composite restorations. The aim of ongoing NIDCR-supported research (DE026122) is to develop antimicrobial composites that physiochemically, mechanically, and biologically outperform the conventional Class V restoratives. Specifically, this project quantifies the antibacterial properties of novel dental monomers (alone or in a polymerized resin matrix) on cariogenic bacteria, Streptococcus mutans. The antibacterial properties of novel monomers were measured using minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) methods. Planktonic S. mutans were cultured (37 °C, 5% CO_2 85% RH) in Todd-Hewitt Broth (THB). S. mutans was exposed to two-fold serial dilutions of monomers suspended in THB with and without 5% fetal bovine serum (FBS). After 24 h exposure, the material suspensions were observed for bacterial growth. Samples with inhibited growth were diluted ≤100,000-fold, spread onto THB-agar plates, and incubated ~24h. The colony forming units (CFUs) were then enumerated. With the MIC assay, some antimicrobial properties were observed in planktonic bacteria, but data suggests that the presence of proteins in FBS shield the antimicrobial potential of the monomer. For example, at the greatest concentration of antimicrobial adhesive 3 (AMADH3), the bacterial effect was reduced significantly ($P<0.05$) in wells containing serum. However, without serum, a greater dose dependent response was observed, where exposure to the greatest concentration AMADH3 yielded approx. 20-fold less S.mutans ($P<0.001$) than wells only half as concentrated. We believe that this collective effort to produce monomers with antimicrobial properties, enhanced miscibility, improved adhesiveness to teeth, and improved coupling with fillers addresses a significant oral health issue associated especially with elderly populations. Its successful completion is expected to yield a new class of restoratives with well-controlled bio-function and a longer service life. Future work will focus on creating monomers with increased surface charge densities to increase antimicrobial properties.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Ha Tran		**Award Number**	70NANB18H153
Academic Institution: University of Maryland College Park		**Major:** Biochemistry	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing either a career in Biochemistry field, or a Master's Degree in Biochemistry		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biomolecular Measurement Division, Bioanalytical Science Group		
NIST Research Advisor:	David M. Bunk		
Title of Talk:	Identification and Quantification of Allergenic Milk Proteins in Food		

Abstract:
The prevalence of food allergy has become an important public health issue and economic concern to the U.S population. A food allergy is an adverse allergic reaction to food which may cause serious health consequences to its patients. As there is no cure or preventative treatment currently exist, the best way to avoid food allergy exposure is strict avoidance. The United States' Food Allergen Labeling and Consumer Protection Act (FALCPA) requires eight major allergens, including egg, milk, peanut, soy, fish, crustacean shellfish, tree nuts, and wheat, to be specifically labeled when being used as ingredients to foods. Regardless of such guidance, the U.S. Food and Drug Administration (FDA) reported that undeclared allergens in food products have continued to be the leading cause of food recalls in U.S. Undeclared allergens in food may result from cross-contamination, poor quality control, mislabeling, or mispackaging during the manufacture. Therefore, it is important for the food industry and regulatory agencies to have reliable methods to identify and quantify food allergens.

As part of the Food Protein Allergen Program at NIST, this project aims on developing a method for identifying and quantifying allergenic milk proteins in food using Liquid Chromatography (LC) and Tandem Mass Spectrometry (MS/MS) after the enzymatic digestion of the proteins into peptides. While LC separates the peptides based on properties such as hydrophobicity and charge, MS/MS provides structural information of those peptides with high sensitivity and molecular specificity. The results of this combined analysis are signals with specific chromatographic retention times and mass-to-charge ratios (m/z), which allow for the detection and quantification of the surrogate peptides of a protein and thus can lead to the identification and quantification of the allergenic protein itself.

In this project, purified milk proteins, including casein (alpha-s1, alpha-s2, beta, kappa) and whey (alpha-lactalbumin, beta-lactoglobulin, and bovine serum albumin), are used as standards for method development. In the future, the method created from this project will be applied on NIST's food-matrix Standard Reference Materials (SRMs) to detect and quantify allergenic milk proteins in those samples.

SURF Student Colloquium

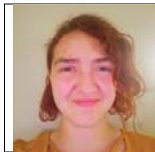
NIST – Gaithersburg, MD

August 7-9, 2018

Name: Julia Trowbridge		**Award Number**	70NANB18H052
Academic Institution: Colorado State University		**Major:** Chemistry	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	I want to go to graduate school and study chemistry or materials science, then work as a research scientist at NREL.		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Nano Materials Research Group		
NIST Research Advisor:	Babak Nikoobakht		
Title of Talk:	Improving the light extraction efficiency of zinc oxide nanofin LEDs		

Abstract:
Zinc oxide (ZnO) nanoLEDs, which could be purposed as lasers for optical sensing devices, have the potential to create new generations of electronic devices because the material has the largest excitation binding energy of all semiconductors. This allows the material to efficiently emit light at higher temperature relative to other semiconductors. It also has a wide bandgap, which allows emission in the ultraviolet spectrum and the ability to tune to shorter wavelengths via bandgap engineering. The nanoLEDs are n-p heterojunction semiconductors grown on a substrate of gallium nitride (GaN). However, GaN presents a challenge in the optical efficiency of the nanoLEDs as it captures about 90% of the generate light due to having a higher refractive index than ZnO. Since GaN is essential to the functionality of the nanowire LED's, the output power of nanoLEDs should be maximized by etching the GaN substrate to microscale pixels to create side facets to refract the light outside, thus increasing the light extraction efficiency of the ZnO nanoLEDs.

For this purpose, I have used a focused ion beam, which shoots a narrow beam of ions to remove atoms from a crystal, to create an etch pattern in the substrate to isolate the nanoLEDs. It was then determined that the structural integrity of the nanoLEDs was intact throughout this etching with surface protection techniques. Dry and wet etching techniques were developed, using a photolithography process to protect the nanoLEDs, to enable a mass scalable process. This final process is expected to make ZnO-GaN nanoLEDs applicable for highly-luminescent nanoscale light sources for a broad range of applications in UV light sources for disinfection, virtual reality displays, lighting applications, and chemical sensing.



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August 7-9, 2018

Name: Makayla Turner		**Award Number**	70NANB18H051
Academic Institution: Boise State University		**Major:** Material Science and Engineering	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Obtaining a Bachelor's degree in Material Science and Engineering and pursuing a career in Science or Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science Division, Materials Structure and Data Group		
NIST Research Advisor:	Eric Cockayne		
Title of Talk:	Interaction of Water with Titanium Oxide Surfaces: A Theoretical Study		

Abstract:
Titanium dioxide (TiO2; Titania) is a white material with many uses such as pigment for paint, food, cosmetics, etc. and as a photocatalyst. One potential application is water splitting, creating hydrogen gas to be harvested for other applications such as hydrogen-powered vehicles. Former theoretical studies assumed the geometry of the Titania surface and the water molecules, whether they be intact or split into OH molecules and H atoms. This summer, we performed an unbiased study of TiO2 + H2O with a combination of density functional theory (DFT) and genetic algorithms. We used a Meta-GGA functional to perform the calculations. This functional uses electron density and the first and second derivatives of that density to calculate the lowest energy state in the molecules and the extended sheet structures. Titania (TiO2), Ti2O3, and water nanosheets were tested separately to find the lowest energy states of each, then tested together to create ternary nanosheet phase diagram. Current testing has shown that in the most stable titanium oxide-water structures, H2O is sometimes intact and sometimes split into OH molecules and H atoms. Surprisingly, the hydrogen left after the water splitting had a tendency to sink below the surface and bond with an oxygen towards the middle of the structure.

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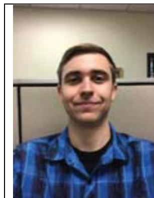
Name: Galen Vincent		**Award Number**	70NANB18H111
Academic Institution: Colorado School of Mines		**Major:** Engineering Physics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue a master's degree in applied statistics.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Polymers Processing Group		
NIST Research Advisor:	Nils Persson		
Title of Talk:	Process Optimization of Blade-Coated Polymer Blend Thin Film Transistors		

Abstract:
Flexible organic field effect transistors (OFETs) made from semiconducting polymers are gaining interest in the world of electronics due to their potential use in applications such as stretchable smartphones and displays. The performance characteristics of these OFETs are impacted by many different factors during the fabrication process, making process optimization a difficult, high-dimensional problem. Use of computer-guided experimental design provides a way to efficiently explore and understand the fabrication variables while systematically improving device performance. In this project, adaptive response surface methodology was used to optimize the performance of thin film OFETs blade-coated from blended polymer solutions of semiconductor DPPT-TT and elastomer SEBS-H1221 in chlorobenzene. Optimization of the active layer material was carried out on non-flexible bottom gate, bottom contact substrates, but the resulting films are elastic, and can be coated onto flexible substrates.

It is common for studies of OFETs to use charge carrier mobility as the only metric for device performance, and while important, it is not the only characteristic of a good device. For this project, a combination of metrics including transfer curve shape and hysteresis, threshold voltage, and mobility were combined into an overall desirability factor for transistor performance. This desirability factor provides a scalar objective that can be optimized with respect to multiple process parameters. Semiconductor solution concentration, blade coating speed, and blade coating substrate temperature were varied, beginning with an initial design space selected based on previous literature work, and using response surface methodology to select subsequent values in pursuit of maximized OFET desirability.

Operable OFETs were fabricated with mobilities ranging from 0.31 to 1.01 cm^2 / V s, threshold voltages ranging from -10.4 V to 0.5 V, and varying values of desirability. Some process conditions lead to blade coat failure and inoperable devices. The knowledge gained from optimization on a lab-scale blade coating system with non-flexible devices should be transferrable to OFET fabrication on large-scale roll-to-roll, fully flexible substrates.



SURF Student Colloquium

NIST – Gaithersburg, MD
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Name: Elijah Williams		**Award Number**	70NANB18H034
Academic Institution: McDaniel College		**Major:** ACS Certified Chemistry	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue a career in chemistry and attend graduate school		
NIST Laboratory, Division, and Group:	Material Measurement Lab, Biomolecular Measurement Division, Bioprocess Measurements Group		
NIST Research Advisor:	Jeffrey Hudgens, Kyle Anderson		
Title of Talk:	Improving the Measurement Quality of Hydrogen Deuterium Exchange Mass Spectrometry		

Abstract:
Measurement quality of biopharmaceuticals is extremely important in assuring drug quality and stability. Hydrogen deuterium exchange mass spectrometry (HDX-MS) is a powerful technique that can be used to measure protein conformational dynamics, thereby facilitating structural and functional characterization of proteins. The technique involves labeling exchangeable hydrogens in a protein with deuterium by incubating the protein in deuterium oxide. The labeling reaction is then quenched by the addition of phosphate buffer at pH 2.5; however, deuterium in amino acid side chains quickly back exchange to hydrogen and only amide backbone hydrogens retain deuterium. Quenched protein samples are subsequently digested on an immobilized protease column into peptides, which are then desalted on a trap column, separated on an analytical column, and measured on a Thermo Orbitrap Elite mass spectrometer. Since protein conformation and dynamics dictate the rate of labeling specific amides, comparison of HDX-MS data from various protein conditions can be used to map binding sites, elucidate mechanisms of action, and assess stability. The goal of this project was to improve the dynamic range of the method by optimizing parameters to reduce back exchange and improve detection. Since temperature impacts back exchange, the temperature of all fluidics and valves after the protease column were reduced from 1 °C to -25 °C. To mitigate freezing at -25 °C, ethylene glycol was added to the mobile phase. The low level of back exchange at -25 °C enabled longer elution gradients, providing greater resolution and signal intensity for peptides. Additionally, electrospray ionization conditions were optimized to reduce in-source back exchange while maintaining sufficient spray stability and ion signal at high concentrations of ethylene glycol. Developing an HDX-MS method that significantly reduces back exchange while improving peptide detection will enable better characterization of pharmaceuticals for both development and regulation.

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August 7-9, 2018

Name: Jordan Winetrout		**Award Number**	70NANB18H086
Academic Institution:	University of Southern Mississippi	**Major:** Polymer Science and Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a PhD in polymer science and engineering		
NIST Laboratory, Division, and Group:	Material Measurement Lab, Materials Science and Engineering Division, Polymer Processing Group		
NIST Research Advisor:	Dr. Alexander Bourque		
Title of Talk:	Predicting Phase Behavior in Organic Photovoltaic Devices		

Abstract:
Organic photovoltaic devices (OPV) are a cheaper and flexible alternative to their inorganic (e.g silicon) counterparts as a source for clean and renewable energy. Reports show OPVs with achievable power conversion efficiencies (PCE) as high as 14%. However, optimization of OPVs has been hindered by the overwhelming parameter space associated with device fabrication. The majority of efficient OPV devices comprise an active layer with a bulk heterojunction (BHJ) morphology which is formed by phase segregation between a donor material and an acceptor material. Previous studies have investigated the BXR donor series for its potential in OPV blends and have shown the BQR (X = Q, quaterthiophene) derivative had the best performance when blended with the fullerene accepter, PC71BM. The focus of this project was to predict phase behavior of BQR blended with non-fullerene acceptor (NFA) materials. Two small molecule NFA series were studied; molecules within each series (ITIC & IDTBR) were differentiated by their side-chains to investigate the effect of chemical architecture on phase segregation. Differential scanning calorimetry (DSC) was used to probe phase segregation by observing melting point depressions in the blends. Spectroscopic ellipsometry (SE) was used to characterize film thicknesses of the blade-coated films. Photoluminescence analysis of the films undergoing thermal annealing was performed to observe morphological changes and identify optimal temperatures for device annealing. Finally, OPV devices comprising each active layer blend were fabricated to determine device performance. It was found that DSC was largely predictive of in-situ PL behavior, but could only partially predict final device performance.

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August 7-9, 2018

Name: Sulan Wu		**Award Number**	70NANB18H084
Academic Institution:	Oberlin College	**Major:** 3-2 Engineering, Biochemistry	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing a career in the biomedical field		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory (MML), Biosystems and Biomaterials Division (BBD), Bioassay Methods Group		
NIST Research Advisor:	Hua-Jun He		
Title of Talk:	Standardization of *HER2* gene copy number variation measurements in liquid biopsy by digital PCR		

Abstract:

Human epidermal growth factor receptor 2 (*HER2*), a member of the epidermal growth factor receptor family, is a breast cancer biomarker that is responsible for approximately 20-30% of breast cancer tumors when its gene is amplified. Liquid biopsy, or a non-invasive biological fluid extraction, is a test that gives insight on the genetic landscape of both primary and metastases, allowing for useful real-time analysis of tumor heterogeneity and dynamics. The accurate measurement of the *HER2* biomarker is critical for diagnostics and proper treatment with anti-*HER2* therapeutics. The challenge, however, is that reliable and accurate measurements of the *HER2* gene copy number variation (CNV) is difficult due to the low presence of circulating tumor DNA (ctDNA) from tumor cells in the background of DNA molecules from normal cells, as well as a lack of standardization. Therefore, the goal of this research is to improve the confidence and reliability of clinical measurements of *HER2* CNV in liquid biopsy by ctDNA reference materials development and analytical validation.

Nucleosomal DNA was prepared from two human breast cancer cell lines: MDA-MB-231, which has a normal *HER2* copy number, and MDA-MB-453, which has a moderately amplified *HER2* copy number. DNA fragmentation was achieved by Atlantis dsDNase treatment to produce lengths like that of DNA found in blood, which is approximately 160 base pairs. Purified nucleosomal DNA were characterized by the Nanodrop, Bioanalyzer, Qubit assay, and polymerase chain reaction (PCR). Highly sensitive digital PCR (dPCR) assays were developed for quantification of *HER2* and 4 reference genes. Gene copy number ratios of *HER2* to the reference genes were used to determine *HER2* CNV by dPCR. The developed ctDNA reference material candidates for *HER2* copy number measurements will be further characterized by next-generation sequencing (NGS). The future interlaboratory study of these reference materials will be performed and evaluated for its utility and communicability. The development of a reference material for ctDNA measurements and analytical validation will allow for improved accuracy in cancer disease management, such as early disease diagnosis, treatment selection, response monitoring, and prognostication.

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August 7-9, 2018

Name: Julie Yagodich		**Award Number**	70NANB18H054
Academic Institution:	Frederick Community College	**Major:** Chemical Engineering and Mathematics	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing a career in chemical engineering or materials science research		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Research Group		
NIST Research Advisor:	Daniel Siderius		
Title of Talk:	Encoding Gas Adsorption Isotherms for Standard Reference Data and Use		

Abstract:

Gas adsorption is of increasing interest to scientists and engineers because of its possible applications in the separation and storage of gaseous mixtures in a cost-effective manner. Adsorption has many notable applications, such as helping the environment by capturing and storing harmful gases, purifying gaseous mixtures, and storing gases for later use as energy sources. An isotherm quantifies adsorption for a material and gas combination. A major drawback with gas adsorption is that each adsorbent exhibits different sorption behavior depending on temperature, pressure, and composition of the gaseous mixture. Because of these complications, extensive reference data is necessary to understand the behavior of adsorbent materials.

The goal of this project is to continue updating the NIST/ARPA-E Database of Novel and Emerging Adsorbent Materials so that more reference data is available for researchers worldwide. Additionally, this project aims to make the database easier to navigate. The database is important because it allows scientists and engineers to access and compare reliable isotherm data. In addition, the database develops a standard for the method by which isotherm data is collected and presented. Many different articles related to gas adsorption are read to find any relevant information. The data, which is either presented as a graph or table, is converted to a self-describing digital format that is entered into the database.

Unfortunately, the current methodology leads to a certain degree of error. There is currently no standard procedure for conducting gas adsorption experiments, which leads to variability in the data. In addition, if a piece of information, such as temperature, is missing from an article, then the entire dataset cannot be interpreted. Finally, when collecting data from graphs, a digitizer is used, which creates a certain degree of error because the user cannot get the exact same data points as the original experimental data.

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August 7-9, 2018

Name: David Yoon		**Award Number**	70NANB18H075
Academic Institution:	Northwestern University	**Major:** Manufacturing and Design Engineering	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Attend graduate school; pursue a career in designing medical devices		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group		
NIST Research Advisors:	Paul Salipante, Steven Hudson		
Title of Talk:	Measuring Viscosity Through a Microliter Capillary Rheometer		

Abstract:

Microfluidic capillary rheometry is an analytic technique often used to characterize properties of solutions. With Newtonian fluids, fluid properties are constant with flow conditions, but non-Newtonian fluids properties can vary with shear rate. The goal of this research is to measure the viscosity of any fluid, using the smallest amount of volume possible. In addition, the measured viscosity of the fluid needs to be constant with varying pressure and flow rate. For example, in applications with biopharmaceutical industries, taking measurements of smaller volumes is cost efficient.

This project focuses on developing and testing a microfluidic device that measures the viscosity of microliter volumes. In this experiment, a pressure controller drives flow through a rectangular or circular glass capillary with well-defined dimensions. This simple and practical design allows for visibility of the cross section of liquid, as well as a template to mount the slide under a microscope. The viscosity is measured using capillary rheology, which relies on measurement of both pressure drop and flow rate through the capillary. The flow rate through the system is measured using calibrated flow sensors and the pressure drop across the entire flow system is assumed to occur across the capillary due to the small dimensions of the capillary compared to the rest of the flow system. Software controls are developed to automate the applied pressure, including reversing the flow direction to limit the volume of fluid used in the experiment. Experiments are automated to measure viscosity over a range of flow rates. Video microscopy allows for further inspection and examination of the fluidic cross section and the motion of the sample interface.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Candace Young		**Award Number**	70NANB18H033
Academic Institution: Chicago State University		**Major:** Chemistry	
Academic Standing (Sept. '18):	Senior at Chicago State University		
Future Plans (School/Career):	Pursue a career in biomedical sciences.		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Chemical Sciences Division, Organic Chemical Science Measurement Group		
NIST Research Advisor:	Christina M. Jones, PhD.		
Title of Talk:	Development of Metabolomics Quality Control Materials for Precision Medicine and Strategies for Forensic Hair Analysis		

Abstract:

Having made contributions to the clinical, forensic, and food industries, metabolomics research involves comprehensive characterization of metabolites in biological systems. This new field of "omics" has been used to better understand altered metabolic processes involved in disease etiology and progression, provide biochemical markers of toxicity, and aid in food authentication. The field of metabolomics is undergoing rapid growth, partly because of the expansion of measurement platforms capable of measuring a broad range of diverse metabolites. Presently, the National Institute of Standards and Technology (NIST) is developing new biofluid-based quality control materials to complement metabolomics measurements applicable to precision medicine while also determining if metabolomic strategies are beneficial to forensic hair analysis. A suite of pooled plasma samples composed of different metabolic health states (i.e., type 2 diabetes, hypertriglyceridemia, and young, healthy African-Americans) were assessed for metabolome differences to determine the feasibility of using the suite as reference materials for harmonization of measurements made by the metabolomics community. Proteins were precipitated from the plasma using organic solvent, and the remaining metabolites were analyzed via liquid chromatography–high resolution mass spectrometry (LC–HRMS). The resultant data was processed, and multivariate analysis techniques were used to explore and analyze the processed data. To determine whether metabolomics can aid forensic hair analysis, hair samples underwent acid hydrolysis to extract metabolites. Hair metabolites were also analyzed using LC–HRMS. Preliminary analysis of the plasma data shows that the phenotypes may indeed be distinguishable, thereby providing evidence that the suite could be used as quality control materials to reduce technical variance in metabolomics studies. However, more work is needed to determine whether metabolomics is beneficial for forensic hair analysis. The hair metabolite extraction and LC–HRMS analysis needs to be further optimized and applied to a test set of different hair samples.

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August 7-9, 2018

Name: Ryan T. Zambrotta		**Award Number**	70NANB18H075
Academic Institution: Northwestern University		**Major:** Applied Mathematics	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursue a Ph.D. in Computational Science		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Material Science and Engineering Division, Functional Polymers Group		
NIST Research Advisor:	Ketan S. Khare and Fredrick R. Phelan Jr.		
Title of Talk:	Atomistic Simulations of the Glass Transition in Small-Molecular Organic Glass Formers		

Abstract:

Many important classes of amorphous materials undergo a phenomenon called the 'glass transition', which involves a change of the material from a high temperature melt state, through a relatively soft and ductile intermediate state, to a final hard and glassy state with a decrease in temperature. Such classes of materials include thermoplastics (e.g., polystyrene, nylon) and thermosets (e.g., epoxy), conventional inorganic glasses, as well as small-molecular organic glass formers (e.g., glycerol, o-terphenyl). Unlike freezing, the glass transition is a more gradual transition over a temperature range to the solid state. Polymers and other amorphous materials are typically processed from the high-temperature melt state (Arrhenius regime), through the non-Arrhenius regime of incipient glass-formation, to the amorphous state below the glass transition. In the non-Arrhenius regime, the dynamics fall out of equilibrium and slow down drastically until at the glass transition temperature (T_g), the material is considered a glassy solid. Curiously, this change in dynamics is not mirrored by a change in the molecular order in the material. Furthermore, T_g is cooling rate dependent property meaning that the faster one cools the melt, the higher the T_g. Altogether, this makes the glass transition phenomenon of extreme interest for both practical engineering applications and scientific fundamentals.

In this project, we perform atomistically detailed simulations of small-molecule glass formers such as glycerol and o-terphenyl. Accounting for rate effects using atomistic molecular dynamics (MD) simulations and making quantitative comparison with experimental measurements has proven to be a difficult task due to the extreme mismatch between experimental and computationally accessible cooling rates which are orders of magnitude faster. As a result, computational calculations of T_g are often more than 100 K larger than those measured experimentally, rendering simulation of little practical value. Therefore, to account for rate effects, we employ and further test the specific volume cooling rate analysis procedure outlined by Khare and Phelan. We will present the volumetric and dynamic behavior of glycerol calculated using the LAMMPS simulation package and the all-atom general AMBER force field (GAFF). Furthermore, we use the time-temperature superposition protocol (TTSP) to present quantitative comparison with experimental results to help bridge the gap between prediction and experiment.

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August 7-9, 2018

Name: Krista Balto		**Award Number**	70NANB18H118
Academic Institution:	University of Delaware	**Major:** Chemistry B.S	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Attend graduate school		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	John Riley Michael Zhang		
Title of Talk:	The Conformation of a Hydrophilic Di-block Copolymer on Silica		

Abstract:

Hydrophilic di-block copolymers, such as polyethylene oxide-poly(2-dimethylaminoethyl methacrylate) (PEO-b-PDMA), can be used to stabilize colloidal dispersions and compartmentalize negatively charged proteins for drug delivery applications. The cationic PDMA block in PEO-b-PDMA can interact with negatively charged drug molecules and particles through electrostatic complexation, while the non-ionic PEO block provides a protective steric layer to prevent particle aggregation and accumulation. In these applications, PEO-b-PDMA in aqueous solution encounters a variety of surfaces, therefore its adsorption mechanism at the solid-liquid interface is important. To understand the adsorption of di-block copolymers, such as PEO-b-PDMA at the solid-liquid interface, we utilized negatively charged silica surfaces as model substrates. Silica was chosen because it possesses a pH-dependent surface charge. When in solution, the non-ionic and cationic blocks adsorb to silica through different mechanisms-- PEO by hydrogen bonding and PDMA by electrostatic attraction. Changes in pH may drive the di-block copolymer into preferred conformations based on the relative strength of these two interactions. Several analytical techniques were used to study the solution adsorption of PEO-b-PDMA on silica: Dynamic Light Scattering (DLS), Quartz-Crystal Microbalance with Dissipation (QCM-D) and neutron reflectometry. DLS measured the charge and size of the silica particles with and without copolymer adsorbed onto the surface, which indicated whether PEO-b-PDMA adsorbed onto the silica particles. QCM-D measured the swelling and mass of the adsorbed layer. QCM-D provided insight into the conformation of PEO-b-PDMA at the solid liquid-interface, but it cannot distinguish the swelling of one block from another. Neutron reflectometry was used to directly determine the conformation of the PEO-b-PDMA layer that adsorbed from solution onto a silica wafer. The PDMA block of the copolymer was deuterated and contrast variation measurements were made to measure the scattering length density profile of the copolymer on the surface at a specific pH. The data yielded through DLS and QCM-D measurements indicated that PEO-b-PDMA adopts a different conformation at pH 4 and pH 10, which was confirmed through neutron reflectometry on the partially deuterated block copolymer. Only through a combination of methods could the conformation of the di-block copolymer be determined, revealing information about the solution adsorption mechanism.

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August 7-9, 2018

Name: Katie A. Behnert		**Award Number**	70NANB18H100
Academic Institution:	Pennsylvania State University	**Major:** Nuclear Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a career in nuclear engineering		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research (NCNR), Reactor Operations and Engineering Group		
NIST Research Advisor:	Marcus D. Schwaderer; Dağistan Şahin, Ph.D.		
Title of Talk:	Physical Components of Secondary Pump Condition-based Monitoring System		

Abstract:

NIST has a nuclear reactor, the National Bureau of Standards Reactor (NBSR), that generates 20 MW of power that is in the form of heat. That heat must be continuously removed to prevent the reactor fuel from melting and for normal operation to continue. This cooling is done by pumping fluid through the reactor core via two separate systems: primary and secondary coolant systems. The primary pumps circulate heavy water - D_2O - through the reactor core itself, then the secondary pumps circulate regular water - H_2O - that cools the heavy water leaving the reactor via an external cooling tower. Both types of pumps have a very important and stressful job, as one can imagine, and preventing them from failing is a top priority. To avoid unexpected failures, condition-based monitoring (CBM) systems can be installed to check the pumps' current status, and perhaps predict failures before they happen.

These CBM systems check the pumps' status in quasi real-time and look for any potential issues that appear to be out of the ordinary. This type of maintenance, where you predict what is going to go wrong before it does, is aptly called predictive maintenance. Looking for potential issues, before they become serious enough to cause failure, is how you keep a critical machine running and prevent unscheduled downtime.

The CBM system that is being designed and implemented in this project is installed on the secondary coolant pumps. This system serves to alert reactor operators if the pumps are exhibiting behavior that is different from the usual. The monitoring is done in two different ways: vibration and temperature analysis. Vibration analysis is done using accelerometers that record the vibrations that the pumps produce. These vibrations are filtered (to take out excess noise) and graphed then - depending on what frequency the vibrations occur at - you can determine what is causing the vibrations, and it can hopefully be remedied. Sometimes, however, the vibration spectra for different faults look similar and a supplementary method needs to be used to differentiate. This supplementary method is called phase analysis. Phase analysis compares the vibrations' waves collected from the sensors (the same ones used for vibration analysis) and uses the phase difference between the sine waves to confirm faults. Each fault has a unique and different phase shift for measurements taken from different axes.

The temperature analysis portion of the CBM system is done by inserting temperature probes into the pumps' bearings oil and watching the temperature's trend over time. As bearings get worn and come closer to failure, the temperature inside them and the surrounding oil increases, so if the temperature begins to rise then it's assumed that the bearing is experiencing a problem and may need to be replaced.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 7-9, 2018

Name: Emily Blick		**Award Number**	70NANB18H153
Academic Institution: The University of Maryland		**Major:** Bioengineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Yun Liu		
Title of Talk:	Exploring the rheological properties of dense lipid vesicle solutions as models for liposomal nanomedicines		

Abstract:
Liposomes are promising candidates for future drug delivery applications due to the similarities in morphology to a cellular membrane. The possibility of developing nanomedicines using phospholipid bilayer vesicles has sparked further investigation of liposomal properties. This study focuses on the rheological and stability properties of two lipid vesicle systems under different conditions. The lipid model system chosen was DOPC, a commonly used research compound for vesicles. The stability experiments were completed over a period of two weeks and tested the impact of vesicle size, solution temperature, and concentration on long term liposome stability. Dynamic Light Scattering was used to estimate the apparent radius of the lipid vesicles and was tested daily to monitor vesicle change over time. Rheology studies were completed to investigate the impacts of steady state shear on liposome deformation and solution viscosity. Also, small-angle neutron scattering experiments were completed to provide insight on vesicle structures and interactions under tested conditions. The clear understanding of the stability and solution properties are key to creating successful nanomedicines. Our experimental results provide new insights on what conditions allow vesicles to remain stable and capable for treatment use. Also, the rheological studies have shown a relationship between steady-shear and solution viscosity and will provide helpful parameters for future medical use.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 7-9, 2018

Name: Hannah Burrall		**Award Number**	70NANB18H080
Academic Institution: Hamilton College		**Major:** Physics and Mathematics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue a career in physics or applied mathematics and/or attend graduate school		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Wangchun Chen, Shannon Watson and Taufique Hassan		
Title of Talk:	Optimization of ^{3}He neutron spin filters for the neutron spin echo spectrometer		

Abstract:
The NIST Center for Neutron Research (NCNR) is developing a new measurement capability, Intensity Modulated Neutron Spin Echo spectroscopy (IMNSE). The new capability requires a compact 3He neutron spin filter (NSF) based polarizer and analyzer with an integrated neutron polarization flipper. 3He gas contained inside a glass cell can be nuclear polarized using spin-exchange optical pumping. The nuclear polarized gas can then be used to polarize and analyze a neutron beam. However, the 3He cell polarization begins to decay once the spin-exchange optical pumping process ends. Thus, a magnetically shielded solenoid is required to supply a uniform magnetic field to maintain the polarization of the cell.

In this study, the magnetic field gradients of the 3He polarizer and analyzer are optimized using a magnetometer field mapping system and the free-induction decay (FID) nuclear magnetic resonance (NMR) technique. The relaxation times (T1) of the polarized 3He cells are measured to characterize the field gradients of the solenoid on the PHADES and NSE beamlines. In addition, a radio frequency (RF) field, orthogonal to the magnetic field produced by the solenoid, is used to invert the 3He polarization using adiabatic fast passage (AFP) NMR. A specially designed sinusoidal RF coil, placed between the main solenoid and a 3He cell, is used to generate an RF signal to invert the spin polarization of the cell. Thus, the neutron spin filer can effectively flip the neutron polarization. The 3He polarization flipping process is optimized using the FID NMR technique and neutron transmission measurements.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Alexa Beatrice Cano		**Award Number**	70NANB18H070
Academic Institution: Texas A&M University-Kingsville		**Major:** Chemical Engineering, Chemistry	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Grethe Jensen		
Title of Talk:	Phase Behavior and Morphology of Microemulsions in a Polymer-Surfactant System		

Abstract:

Microemulsions are thermodynamically stable systems of oil, water, and surfactant. The nanoscale structures of such mixtures are crucial for predicting and understanding the macroscopic properties of the microemulsion, such as rheological behavior. However, much is still unknown about the phase behavior and subsequent structures of specific microemulsion systems. In this study, a member of a commercially available class of polymeric surfactants known as Pluronics was chosen for further investigation of such nanostructures at high copolymer concentrations as a function of temperature and shear. Pluronics are nonionic triblock copolymers composed of a hydrophobic central polymer chain adjoined on each side by hydrophilic polymer chains. The highly amphiphilic nature of Pluronics allows for their self-assembly and rich lyotropic liquid crystalline phase morphology in selective solvents. In this study, samples were prepared at 40, 60 and 70 wt% copolymer compositions and varying water:oil ratios. Visual inspection was first used to map the phase diagram of Pluronic P84 in water and p-xylene as a function of temperature. Small angle neutron scattering (SANS) was used to verify the phase behavior and corresponding structures of the samples over a temperature range of 25°C to 75°C. SANS measurements were also used to calculate the interspatial distances of the lyotropic liquid crystalline phase packing structures. This data was compared against the volume fraction ratios to propose geometric and thermodynamic explanations for the observed phase behavior. Rheological measurements were also performed as a complementary method to characterize and understand the microstructural properties of the observed phases. Small amplitude oscillatory shearing was utilized to probe the relationship between the equilibrium mechanical properties and the structural properties of the microemulsions. By combining rheology and SANS, we were able to identify hexagonal, bicontinuous, lamellar, and micellar phases in our polymer-surfactant system, as well as thermally control the transitions between these phases at high polymer concentrations.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9 2018

Name: Omar Cavazos		**Grant Number**	70NANB18H070
Academic Institution: Texas A&M University-Kingsville		**Major:** Mechanical Engineering (Nuclear Engineering & Mathematics Minors)	
Academic Standing (Sept. '18):	Graduate Student in Engineering Technology at University of North Texas		
Future Plans (School/Career):	I will ultimately pursue a PhD in Mechanical Engineering and would like to work at a national laboratory.		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research (NCNR), Reactor Operations and Engineering Group		
NIST Research Advisor:	Dagistan Sahin		
Title of Talk:	NBSR Thermodynamic Performance Analysis		

Abstract:

National Institute of Standards of Technology (NIST) has a 20 MW, heavy water moderated nuclear reactor (NBSR: National Bureau of Standards Reactor). During normal operations, the secondary cooling water outlet temperature is maintained between 90 °F to 96 °F, which is below the outside temperature, specifically in the summer months when temperatures exceed 100 °F. This negative temperature difference significantly reduces heat transfer through the cooling towers, resulting in an underutilized cooling system. The cooling tower effectiveness can be significantly improved by increasing the cooling tower secondary water temperature.

A model of the reactor cooling system was developed to analyze various process parameters to improve the calorimetric performance of the NBSR and calculate the optimum safe operating temperatures. The proposed changes will substantially increase the operational band of the secondary cooling system resulting in optimized process performance. Optimization will also result in energy savings. The cooling towers consume about 300 kW at high setting, at approximately $0.1 per kWh, this equates to $21,600 per month. If only 3 cooling towers were used at low setting, power consumption would be reduced to approximately 78 kW, corresponding to $5,600 per month. Considering only the warmer months, savings would be approximately $80,000 per year.

Simulink software in conjunction with the Thermolib add-in was selected to develop the thermodynamic model, which includes components such as cooling towers, heat exchangers, and pumps. The optimization analysis was conducted by varying environmental temperatures, secondary loop flow rates, and secondary cooling water temperatures. The data produced from the model was compared to historical NBSR data. Overall, this thermodynamic analysis will greatly benefit the operation of the NBSR for years to come by reducing the impact of environmental/weather conditions on the performance of the NBSR.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Joshua Devorkin		**Award Number**	70NANB18H066
Academic Institution: University of Illinois Urbana-Champaign		**Major:** Nuclear and Plasma Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Planning on attending graduate school for plasma-material engineering focused on biomedical research		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Dr. Susana Teixeira and Dr. Yimin Mao		
Title of Talk:	Cellulose under pressure for new biopolymers		

Cellulose is an abundant biopolymer occurring in high plant, wood and cotton, but can also be synthesized by some types of bacteria and algae. Intrinsically by the natural biosynthesis process, cellulose molecules crystallize to form nanofibers/crystals, the basic structure of microfibrils. Further aggregation allows the formation of macro-fibrillar bundles which provides the basic backbone to a cell's mechanical strength. These cellulose nanofibers (CNF) serve as a fundamental building block for new materials and have a wide range of applications in antimicrobial films, biomedical implants, templates for electronic components, water purification and many others. However, to extract the nanofibers harsh chemical treatment processes such as the TEMPO-mediated oxidation reaction are needed limiting the efficiency of the reaction and industrial usage because of the toxicity and price. Therefore, the aim of this study is to investigate how high hydrostatic pressure can be used to increase the efficiency of the reaction while decreasing the need for harsh treatments. In parallel, there is an increasing need for characterizing the dimensions of the nanofibers from the nanoscale to microscale in solution, that the conventional microscopy techniques cannot measure. Small-angle neutron scattering (SANS) carried out on NGB 30m determined cross-sections of the individual nanofibers. Atomic force microscopy (AFM) confirmed the accuracy of the scattering data from images taken in real space. SANS data revealed that applying high hydrostatic pressure increased the rate of oxidation and decreased the concentration of reagents needed for extraction producing long nanofibers. High pressure treatment is therefore an economically friendly method for enhancing this green process to break down the cellulose. The resulting high aspect ratios of CNF's suspensions make them relevant to produce novel new materials with applications in thin films and hydrogels, with a much lower concentration of cellulose needed.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Samantha Isaac		**Award Number**	70NANB18H064
Academic Institution: West Virginia University		**Major:** Physics & Mathematics	
Academic Standing (Sept. '18):	Graduate Student @ University of Illinois, Urbana-Champaign		
Future Plans (School/Career):	Attending University of Illinois, Urbana-Champaign for a Physics Ph.D		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group.		
NIST Research Advisor:	Leland Harriger		
Title of Talk:	Monte-Carlo Exploration of Focused Neutron Guide Geometries		

Abstract:
A new cold neutron source will soon be installed at the NIST Center for Neutron Research (NCNR). At this time, the current cold triple axis spectrometer, SPINS, and its neutron guide, NG5, will also be redesigned in order to increase data collection by at least one order of magnitude. Currently SPINS is fed by an older generation straight, rectangular guide with Ni58 coating. Newer supermirror guide coatings can greatly increase neutron acceptance, but at a cost of lower reflectivity. Using Monte Carlo simulations, we have developed a double focusing guide and monochromator that produced a factor of seven increase in intensity at the sample position. Taking this new primary spectrometer as our baseline we have explored two modifications to further improve performance. The first is a removable SELENE tip option that theoretically offers extremely fine beam masking capability down to 1mm and simultaneous variable control of the beam divergence. The second is a full redesign of the primary guide based on a kinked double ellipse that breaks line of sight. The findings for these two modifications will be discussed.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Paul Neves		**Award Number**	70NANB18H153
Academic Institution:	: University of Maryland, College Park	**Major:** Physics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a PhD in Physics		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Nick Butch, Juscelino Leão		
Title of Talk:	All Tied Up in Knots: Skyrmions in Chemically Substituted Cu2OSeO3		

Abstract:
In certain non-centrosymmetric magnetic systems, an applied magnetic field can create small spin vortices known as magnetic skyrmions. These structures could potentially be used in future spintronics data storage, and offer interesting insights into the fundamental physics within magnetic materials. Cu2OSeO3 has recently received significant attention as the only known multiferroic skyrmion material. Magnetization measurements suggest that chemical substitutions in this compound have a strong effect on the skyrmion phase. Here, I will discuss our efforts to characterize the structure and dynamics of skyrmions in various chemical substitutions of Cu2OSeO3 using magnetometry, wavelength-dispersive spectroscopy, X-ray spectroscopy, and small angle neutron scattering (SANS) in various static and dynamic magnetic fields from 60 K to 12 K.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

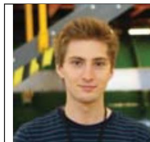
Name: Temiloluwa Okusolubo		**Award Number**	70NANB18H101
Academic Institution:	University of Maryland, Baltimore County	**Major:** Biology	
Academic Standing (Sept. '18):	Senior at the University of Maryland, Baltimore County		
Future Plans (School/Career):	Pursuing an MD-PhD to become a clinical researcher		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Michihiro Nagao, Elizabeth Kelley		
Title of Talk:	Correlating Gramicidin Ion-Channel Formation to Artificial Membrane Dynamics		

Abstract:
Cell function and disease have a direct link to nanoscale membrane dynamics and macroscopic structure. Numerous studies have found that changes in membrane characteristics such as fluidity and thickness correlate to how different sub-types of somatic cells respond to changes in their environment. Investigating the effects of different conditions on membrane dynamics is therefore important to understanding both biological membranes and cellular function. Qualitative and quantitative analyses of membrane structure and dynamics reveal some of these resultant effects. Neutron scattering techniques reveal structural characteristics in sub-nanometer to tens of nanometers scales. Dynamic features in picoseconds to hundreds of nanoseconds timescales can also be observed. Together these techniques allow us to examine the structure and motion of 5 nm thick lipid membranes. Past experiments using small angle neutron scattering (SANS) and neutron spin echo spectroscopy (NSE) have given insight into membrane response to the presence of protein. In this study, the response of unilamellar vesicle membranes to the addition of increasing amounts of a well-characterized ion-channel protein – gramicidin – is further analyzed. Artificial vesicles composed of membranes containing varying amounts of gramicidin and a lipid of interest are created via extrusion. Samples are pushed through filters of decreasing pore size to ultimately obtain vesicles that are 100 nm in diameter. With the use of dynamic light scattering (DLS), a technique used to determine the size distribution of suspended particles in solution, the size of the vesicles is confirmed. Density measurements are utilized to carry out quantitative characterization. This measurement is done to specifically look at lipid behavior over a chosen temperature range. An assay based on measuring the time-course of fluorescence quenching from fluorophore-loaded large unilamellar vesicles (LUVs) due to entry of a quencher through the gramicidin channels; is performed to establish that the protein is being incorporated into the vesicles. These investigations collectively serve to correlate channel formation to membrane dynamics. While the previously mentioned techniques only provide information on a much larger scale, SANS and NSE experiments allow us to probe the membrane at a nanoscale level. SANS provides us with data from which information about the structure of the membrane can be gleaned. Of particular interest to us is the formation and orientation of the gramicidin channels as well as channel-membrane interactions. To understand more about the dynamics of the membranes, NSE was used. NSE allows for aspects like height fluctuations, stretching, and bending in the membrane to be extracted. Together this data provides a more detailed explanation of how proteins might influence membrane activity on a biological basis, therefore influencing a cells activity.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 7-9, 2018

Name: Zach Riedel		**Award Number**	70NANB18H141
Academic Institution: Clemson University		**Major:** Materials Science & Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue research and development in industry		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Katie Weigandt, Ryan Murphy		
Title of Talk:	Capillary µRheoSANS for High Shear Rate, Low Volume Studies		

Abstract:
At high shear rates, complex fluids often undergo important microstructural changes such as alignment and degradation. While traditional rheometers can reveal shear-induced structural changes when combined with small angle neutron scattering (SANS), they often cannot reach desired shear rates for industrial applications and require fluid volumes impractical for expensive samples. To combat these concerns, we designed the capillary µRheoSANS with small volume silica capillaries together with high pressure pumps to produce wall shear rates as high as 10^6 s^{-1}. Newtonian water-glycerol mixtures were used to calibrate the capillary µRheoSANS and to determine the instrument's viscosity, flow, and shear rate limits. After the calibrations, Non-Newtonian wormlike micelles with well-characterized, flow-induced structural changes at moderate shear rates were studied with the capillary µRheoSANS. The two samples contained differing surfactant amounts in a NaCl-D_2O brine. Alignment was observed for both at flow rates as low as 0.01 mL/min with higher values for the more viscous, higher surfactant sample. With increasing flow, both samples experienced increasing alignment up to a critical point where decreasing and nonmonotonic alignment with increasing shear rate could indicate instabilities or microstructural changes. The experiment notably required only 2 mL of sample and reached shear rates up to $4{\cdot}10^5$ s^{-1}.
Subsequent experiments involving a star polymer and the NIST standard monoclonal antibody demonstrated the versatility of the capillary geometry. These measurements prove the viability of high shear rate, low sample volume neutron scattering using capillary µRheoSANS.



SURF Student Colloquium
NIST – Gaithersburg, MD
August 7-9, 2018

Name: Kirill Stakhovsky		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Computer Science	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Entering the workforce, software development		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Reactor Operations and Engineering Group.		
NIST Research Advisor:	Dr. Sahin, Dagistan		
Title of Talk:	Operating a Virtual Nuclear Reactor using HoloLens Technology		

Abstract:

The control system of the National Bureau of Standards Reactor (NBSR) is under the constant process of being upgraded. 3D model and 2D technical drawings of the Human Machine Interface (HMI) were previously designed as part of the renovation process. However, there is a great need for a tool that specializes in training the reactor operators.

Augmented Reality is a new technological tool that changes a user's perception of the world around them by projecting realistic Holograms onto physical surfaces. Using Microsoft HoloLens technology and the Unity 3D game engine, I created an application that depicts a realistic portrayal of the reactor console for training and simulation. The simulator enables extensive safety and operational training to reactor operators. For instance, the initial set of scenarios include "Fire on the console", "Reactor startup", "Loss of Coolant" etc. The simulator will further allow engineers to present design changes to the operators before implementation.

My project involved taking existing 3D model drawings and reproducing it in the Unity 3D environment so it can deploy to HoloLens. This involved using the game engine to model, configure, create and manipulate objects to piece together a fully virtual, holographic and working reactor console, all confined in a small headset, ready to be deployed and operational in any environment. This has significant advantages when compared to traditional training modules and simulators. The small size and weight of the Hololens Device is less cumbersome than building a physical apparatus. The ease of use of Unity Game Engine allows programmers to envision and produce countless amounts of activities, scenarios and lifelike experiences. Augmented and Virtual reality technologies are still in their infancy, but because of their innate advantages, they will see much use in the future.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Carrie Stemple		**Award Number**	70NANB18H063
Academic Institution: Wilson College		**Major:** Veterinary Medical Technology: Biology	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing a bachelor's degree in Veterinary Medical Technology, testing to become a certified veterinary medical technologist, pursuing a career as a CVT.		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Amy Xu PhD		
Title of Talk:	Characterizing Adjuvant-Protein Interactions During Freeze-Thaw Cycles		

Abstract:

Adjuvants are the key components in vaccines, they are a class of substances included in a vaccine formulation to boost the immune responses against the specific antigen. It is known that adjuvants and antigens interact in vaccines and the body but the exact way that they interact is not clear. The only approved adjuvants for use in the United States are Aluminum-based. Therefore, this project is meant to develop understanding about how aluminum adjuvants and antigens interact by characterizing the microstructures of model protein-aluminum adjuvant complexes with contrast-matching small angle neutron scattering (SANS). It is expected that the use of differential scanning calorimetry (DSC) will provide insight about how tightly the protein and adjuvant bind. That will be important because it has been found in earlier studies that how tightly the protein and adjuvant bind affects the efficacy of the vaccine. Additionally, the effects of freeze-thaw cycles on their interactions will be characterized with multiple techniques. The results will help to define how the components of vaccines interact, the temperatures at which it is safe to store vaccines, and how additives can be used to stabilize the vaccines to allow a greater range of temperatures to be safe for vaccine storage.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Greg Suczewski		**Award Number**	70NANB18H082
Academic Institution: Middlebury College		**Major:** Physics and Mathematics	
Academic Standing (Sept. '18):	Junior @ Middlebury College		
Future Plans (School/Career):	Pursuing PhD in theoretical physics		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Paul Kienzle		
Title of Talk:	Incorporation of the Beta Approximation in SASView		

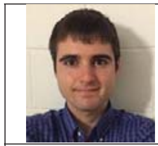
Abstract:

Small Angle Neutron Scattering (SANS) is a common technique used to study the structure of soft matter materials and the interactions between nanoparticles in a solution. During an experiment, neutrons are directed through a sample of interest, where they are scattered due to their wave characteristics. Since the scattering pattern is affected by the shape, size, and relative positions of the particles, it can be analyzed to determine the sample's molecular mass, aggregate mass, aggregate size, protein-protein interaction, phase transition, and fractal structure.

SASView is one of the most popular data analysis programs for studying SANS. It simulates a variety of scattering patterns based on various parameters and models, including spheres, ellipsoids, and cylinders. Existing code only handles the cases of dilute polydispersed solutions (anisotropic and/or anisometric particles) and dense monodisperse solutions (isotropic and/or isometric particles); It cannot be used to study dense colloids like milk, shampoo, red blood cells, or body armor. Therefore, the goal is to improve SASView with the so-called beta approximation theory, which can produce more precise results for dense colloids.

The beta approximation, developed many decades ago, accounts for neutron interaction with isotropic/anisotropic particles of varying size, assuming the particle size and orientation is uncorrelated with position. Adding this method to SASView will require foundational changes to SASView's calculation engine and user interface. Many of SASView's theoretical models will need to be updated. The incorporation of the beta approximation into SASView will enable scientists worldwide to study their materials more accurately. It can also benefit scientists working at synchrotron sources who use small angle x-ray scattering to study their materials.

Future adjustments to SASView include improving the precision of numerical integration techniques and adding alternative calculation methods, such as the local monodisperse approximation, partial structure factor, or scaling approximation of partial structure factor.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Ryan Underwood		**Award Number**	70NANB18H117
Academic Institution: University of Central Florida		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a career in Mechanical Engineering while getting my graduate degree in Mechanical Engineering/Thermo-Fluids		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Thomas Gnaupel-Herold		
Title of Talk:	Determination of crystallite orientation distribution function (ODF) from neutron diffraction data		

Abstract:

The NIST Center for Neutron Research is currently upgrading the capabilities of the BT8 Stress and Texture diffractometer to the effect of a massive increase (x 30) in performance and amount of data generated. A proportional increase in data processing capability, specifically for the analysis of texture data, is necessary and specific computer codes need to be developed to allow quasi-real-time processing. Texture in a material is when a grain structure shows a preferred orientation, also called crystallographic texture. This is a result of thermo-mechanical processing and its interaction with the crystal structure of the constituent grains. Crystallographic texture allows for the identification of the material's anisotropic properties, which is why the study of texture is critical to material manufacturing. Pole figures are experimental data that represent the density of grain orientations in polycrystalline materials. If two or more pole figures are gathered, it is possible to construct a complete three-dimensional statistical description of the texture, called the crystallite orientation distribution function (ODF). ODF data are crucial for the prediction of both elastic and plastic properties of materials. Several approaches for ODF calculation from pole figure data exist, with the use of generalized spherical harmonics as one of the best documented methods. The documentation includes both numerous scientific publications and some computer code in Fortran IV. The main objective of this project was to transcribe the published Fortran code, which was originally written on punch cards and magnetic tapes, into a modern Fortran 95 language. Modernizing and optimizing the code to compile and run on a Fortran 95 complier is the immediate objective. Once fidelity of the calculations is verified through comparison with published results the code will be transcribed into the Delphi language for integration in the existing code base for neutron data analysis and simulation.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Abdullah Weiss		**Award Number**	70NANB18H070
Academic Institution: Texas A&M University-Kingsville		**Major:** Mechanical Engineering	
Academic Standing (Sept. 2018):	Graduate Student in Nuclear Engineering at Texas A&M University		
Future Plans (School/Career):	Short term: I will be working on my PhD in nuclear engineering starting this fall Long term: I would like to work at a national laboratory		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Reactor Operations and Engineering Group		
NIST Research Advisor:	Dagistan Sahin, PhD; Marcus Schwaderer		
Title of Talk:	Digitization of a Secondary Pump Condition-based Monitoring System		

Abstract:

A condition-based monitoring system was designed and developed for usage in predictive maintenance of the secondary pumps for the National Bureau of Standards Reactor. The system relies on vibration and temperature signatures from the pumps to continuously analyze any abnormalities and monitor their health. In this project, a MATLAB program was developed to control, display, interpret, and analyze the vibration and temperature data in quasi-real-time (updating every 30 seconds).

The raw vibration data are averaged every 30 seconds and used to determine the overall vibration quantity using industry-standardized measures. The same raw data are also passed through a Fast-Fourier Transform filter, and an average spectrum of the past 30 seconds is computed and displayed for further analysis. The program utilizes a custom method to detect relevant peaks, which it then uses to assess the health of the pumps. Upon finishing its assessment, the program displays color-coded predictions about potential conditions it detected, including misalignment, mechanical looseness, oil whirl instability, flow turbulence, and cavitation. The program also includes phase analysis capabilities. The historical temperature measurements are also averaged and plotted. The program alerts the user about high temperatures based on user-defined temperature limits.

The entire program is displayed using a relatively intuitive tabbed graphical user-interface that includes a settings tab, a summary tab, and a tab for raw and filtered vibrations spectra for each of the vibrations input channels. Such a program and system allows for increased system reliability, and increased financial savings in operational and maintenance costs, and automates detailed spectral analyses, which saves time as well. For those reasons, the developed system and program have been installed on the secondary pumps, with plans of being installed on the primary pumps as well.

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NIST – Gaithersburg, MD

August 7-9, 2018

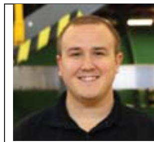
Name: Aubrie Weyhmiller		**Grant Number**	70NANB18H071
Academic Institution: Rowan University		**Major:** Biophysics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursing a Graduate Degree in Health Physics		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research (NCNR), Health Physics and Reactor Operations and Engineering Groups		
NIST Research Advisors:	Tim Barvitskie, Danyal Turkoglu		
Title of Talk:	Online Platform for Radiological Computations		

Abstract:

The NIST Center for Neutron Research (NCNR) is a national user facility with over 2,000 participating staff, research associates and guest users annually. Neutron-based measurements contribute to a broad spectrum of activities including engineering, materials development, polymer dynamics, chemical technology, medicine and physics. An unintended consequence of such measurements are the prompt gamma emissions and induced radioactivity due to neutron activation. When performing sample measurements, it is important that individuals do not receive any unnecessary radiation exposure and their doses are maintained "as low as reasonably achievable" (ALARA). Knowledge of the potential doses can be advantageous in planning work activities and minimizing personnel exposure.

Various desktop programs exist that perform such calculations; unfortunately they only perform a limited number of calculations and the results are not presented in a useful format. An online platform that performs bounding dose calculations and presents the results in a user-friendly format was developed as screening tool to alert NCNR users and Health Physics staff of potential doses from experimental samples. Calculations performed by the program include: maximum external unshielded dose rates from prompt and specific gamma emissions from activation products, maximum direct contact skin dose rate, and maximum internal dose from inhalation and ingestion.

The platform utilizes data and reports from the International Commission on Radiological Protection (ICRP), the Nuclear Regulatory Commission (NRC), and a *Health Physics* journal publication. The application is written in Python and runs locally on various web browsers. Possible future additions include decay calculations using the Bateman equation, dose calculations of various sample geometries, and MCNP Source Card definitions. Presently, this online platform will provide the NCNR users and Health Physics group with a screening tool for potential doses. There is potential for this application to be deployed on a server and utilized by groups in other neutron facilities.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Caleb Wigham		**Award Number**	70NANB18H142
Academic Institution: Texas Tech University		**Major:** Chemical Engineering	
Academic Standing (Sept. '18):	Graduate Student at Rensselaer Polytechnic Institute		
Future Plans (School/Career):	Pursuing a career as a research scientist		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Ryan Murphy		
Title of Talk:	Crosslinking silica-based nanoporous networks under ambient conditions		

Abstract:

Nanoporous solids have excellent physical and chemical properties and show great promise in separations, catalysis, insulations, and hydrophobic coatings. In particular, silica-based networks are characterized by their low density, high porosity, and thermal stability. However, the brittleness of porous silica networks often leads to cracking as a result of strong capillary forces during solvent evaporation. Supercritical or freeze-drying methods circumvent this problem, but at the expense of additional synthesis steps, increased energy demand, and scalability problems. The current work is focused on synthesizing robust silica networks using ambient drying conditions. The free-radical polymerization of diisocyanates, block copolymers, and silica nanoparticles is found to improve structural integrity and increase flexibility of the material. The composite microstructure is probed with small-angle neutron scattering, providing detailed information about the particle size and distribution, the oligomer structure, and the homogeneity of the polymer additive. By varying the concentration of block copolymers and crosslinking particles in our system, we aim to solve the optimization challenge of minimizing the polymer additive while promoting high porosity, low density, and low thermal conductivity.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Abigail Wilson		**Award Number**	70NANB18H067
Academic Institution: Tufts University		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Sophomore, Tufts University		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Dr. William Ratcliff		
Title of Talk:	Applying Reinforcement Learning to the Determination of Crystal Structures with Neutron Diffraction		

Abstract:
The properties of materials are determined by how their atoms are arranged. Neutron diffraction is a key tool in determining the structure of crystals. However, there are a limited number of neutron sources and limited time is available for performing these crucial measurements. The goal of this project is to optimize the process of taking neutron diffraction measurements for crystallography. We applied Reinforcement Learning techniques to the task of learning which neutron diffraction measurements are most important to an accurate determination of a crystal's structure. Reinforcement Learning agents interact with a defined environment in which they can decide which actions to take and are told how well they are performing with a reward. In this case, the agent chooses what measurements to make for a given crystal and then receives numerical feedback on how well its decision improved the model of the crystal. In this talk, I will discuss the performance of various reward functions and some of the strengths and weaknesses of Reinforcement Learning in this problem space.

PML

Last Name	First Name	Lab
Alberts	Gabriel	PML-Elec Engr
Arp	Gabriela	PML-Elec Engr
Borres	Jeffrey	PML-Elec Engr
Chavali	Sai Meghasena	PML-Elec Engr
Croley	Rhett	PML-Physics
Damazo	Isabel	PML-Elec Engr
Dee	Alana	PML-Elec Engr
Doris	Michael	PML-Physics
Eckardt	Benjamin	PML-Physics
Fu	Matthew	PML-Elec Engr
Ho	Kevin	PML-Elec Engr
Isele	Erik	PML-Physics
Kirsch	Dyland	PML-Physics
Malin	Merrik	PML-Elec Engr
Manasiya	Siminben	PML-Elec Engr
May-Pohlman	Laurelia	PML-Elec Engr
McLaurin	James	PML-Physics
Meek	Stephen	PML-Physics
Mullins	David	PML-Physics
Murthy	Vaishnavi	PML-Elec Engr
Orban	Peter	PML-Physics
Sarwat	Sumaiyah	PML-Elec Engr
Schmale	Henry	PML-Physics
Siegel	Jacob	PML-Physics
Sredenschek	Alexander	PML-Elec Engr
Stauffer	Eileen	PML-Physics
Todd	Alexander	PML-Physics
Wages	Hunter	PML-Physics
Walz	Francis	PML-Elec Engr
Wernsing	Galahad	PML-Physics
Whiting	Zachary	PML-Physics

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Gabriel Alberts		**Award Number**	70NANB18H131
Academic Institution: University of Florida		**Major:** Physics, Music	
Academic Standing (Sept. '18):	Postbaccalaureate		
Future Plans (School/Career):	Applying to graduate school for various acoustics-related projects		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, Dimensional Metrology Group		
NIST Research Advisor:	Dr. Meghan Shilling		
Title of Talk:	PrediCTing Errors: Test Method Development for CT Systems		

Abstract:
X-ray computed tomography (CT) is a widely used, non-destructive method to obtain volumetric information about objects. CT systems use a focused beam of x-rays to penetrate an object and produce an intensity profile dependent on material attenuation properties. Although most well-known for its use in medical imaging, x-ray CT is also an important tool for material analysis and dimensional metrology because external and internal structures can be studied. We are developing test methods for the performance evaluation of CT systems for dimensional metrology that will contribute to the ISO 10360 series and ASME B89 series of performance standards. The Dimensional Metrology Group has developed models to predict how various geometric errors in the CT system affect form and length measurements on an artifact. These models use radiographs obtained from aRTist – a detailed CT simulation software – and the commercial system's reconstruction software. This project validated several of these models with radiographs obtained from the system using a physical reference artifact and the same reconstruction software. Measurement results of the reference artifact with no introduced error were compared to those where an error from either detector tilt, an unstable magnification axis, or an unstable rotation axis was introduced. The model's predictions should correspond to the differences in form and length measurements between these two cases. By observing the correlations between the simulations and physical measurements, we validated the simulation methodology used for multiple error sources.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Gabriela Arp		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Public Health Science	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Optical Radiation Group		
NIST Research Advisor:	Maritoni Litorja		
Title of Talk:	Spectral Analysis of Glycated Hemoglobin		

Abstract:
Blood glucose levels provide information on the body's level of efficiency regarding the digestion of glucose and whether the compounds like insulin and glucagon are functioning properly. Any excess glucose, not used or processed by the body, gets taken up by hemoglobin to create glycated hemoglobin, HbA1c. The average person has below 42mmol/mol (6%) HbA1c and a diabetic will have 48mmol/mol or above (6.5%>). Safe blood glucose levels, upon waking up, fall between 3.9-5.6 mmol/L and after consuming a meal rise to 3.9-7.8 mmol/L. It becomes a concern and an indication of either type I or type II diabetes when the individual's levels rise to 4-7 mmol/L before a meal and up to 9 mmol/L after eating. To monitor these numbers- both ones own and at a healthcare facility- a finger is pricked using a lancing device and the blood is transferred onto a test strip which gives glucose level results. This method is invasive, painful and wasteful. As a promising alternative, a non-invasive optical sensor has been a topic of much discussion. This noninvasive measurement of blood glucose needs to be inexpensive so that the visible and near-infrared spectral regions will be used. To be able to observe blood glucose non-invasively, the spectral changes in this region need to be understood. To further research on this topic, testing is being performed to observe spectral responses when excess glucose is added to hemoglobin solution. It is expected that looking at the different spectral regions- blue, green, red and near infrared- that some regions may change with their glucose reaction compared to that without glucose. This will lead to qualitative observations and quantitative estimates based on the change in spectral absorbance and its significance in the clinical setting.

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August 7-9, 2018

Name: Jeffrey Borres Martinez		**Award Number**	70NANB18H128
Academic Institution: Universidad del Turabo		**Major:** Electrical Engineer	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursing a M.S. and PhD on power electronics, control system, or computer sciences after graduating the University of Turabo.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Mass and Force Group		
NIST Research Advisor:	PhD. Gordon Shaw		
Title of Talk:	Robotics mass exchange for advanced metrology		

Abstract:
The kilogram is the last artifact and will be redefined soon this year. As for now, the standard is a Platinum-Iridium cylinder that is changing as the time passes. To fix that problem the new standard would be a natural constant that will be measured with electrical and dimensional metrology using specialized balances that can realize mass at the level of kilograms to milligrams and below. Still the mass artifacts calibrated on the balances will be in used to distribute the standard. Performing a calibration with very small mass artifacts can be critical. The automated balances are used to reduce the measurement uncertainty. Here we report the work done on both vacuum and air balances. First the electrostatic force balance (EFB) was modified and then a new version of the automated air balance was developed. One of the limitations on the accuracy of the EFB mass measurements is the stability of the materials that compose the mass artifact, so it is desirable to make multiple measurements to ensure the artifact stability. The automated mass exchange design was improved to eliminate the possibility that a mass holder could damage the balance. The automated air balance will make life easier since it going to be doing the measurement on its own, but a new carousel and mass holders are required to improve its movement and safety. A new control system was also developed in LabVIEW. At the end we should have an entirely new automated balance for mass measurement in air and an improved EFB that will help NIST with the measurement process for the new kilogram definition.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Sai Meghasena Chavali		**Award Number**	70NANB18H153
Academic Institution: University of Maryland College Park		**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Graduate Student at University of Maryland College Park		
Future Plans (School/Career):	Attending graduate school at the University of Maryland College Park		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Radiation Physics Division, Neutron Physics Group		
NIST Research Advisor:	Shannon Hoogerheide		
Title of Talk:	Systematics in the Neutron Lifetime Measurement		

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). Measuring the neutron lifetime using the beam method requires precise measurements of the number of neutrons in the beam and the number of protons resulting from neutron decay inside a well-known trap volume. To understand systematics, we need to know how these values are affected by changes to a wide range of experimental parameters and we need to confirm that they do not change over time. In my talk, I will present an overview of the beam lifetime experiment. I will describe the apparatus I put together for measuring neutron flux along with a comparison of recent and older flux measurements. I will also discuss some of the data analysis I performed to examine how the proton rate (and thus the extracted neutron lifetime) is affected by changes to some experimental parameters. Additionally, I will show some images of the neutron beam distribution.

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August 7-9, 2018

Name: Rhett Alston Croley		**Award Number**	70NANB18H136
Academic Institution: University of Kentucky		**Major:** Mathematics/Physics	
Academic Standing (Sept. '18):	Junior at the University of Kentucky		
Future Plans (School/Career):	Attend graduate school for pure math or mathematical physics		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Physical Measurement Laboratory, Neutron Physics		
NIST Research Advisor:	Hans Pieter Mumm		
Title of Talk:	Data Analysis of the Alpha-Gamma Neutron Monitor Technique		

Abstract:

Accurate counting of slow neutrons is important to variety of fields. Applications that are of particular interest here at NIST are the determination of the lifetime of a free neutron and the measurement of standard neutron cross sections and branching ratios. The neutron lifetime, for example, determines aspects of matter formation in the early universe. For in-beam neutron lifetime experiments, like those being performed at NIST, a precision measurement of the neutron flux monitor efficiency is crucial to achieving a one second neutron lifetime measurement. Currently, a transfer calibration method called the Alpha-Gamma technique is being used to measure the neutron flux in the NG-6m beamline. This technique allows the detection efficiency of two HPGe gamma detectors to be calculated from the measured absolute decay rate of a well-known Pu-239 source. It has been demonstrated that this technique allows for the determination of the detection efficiency of the flux monitor to an unprecedented accuracy of better than 0.1%. Presented, are the results and error analysis for the calibration of the neutron monitors being used in the NG-6m beamline experiments at NIST.

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August 7-9, 2018

Name: Isabel Damazo		**Award Number**	70NANB18H132
Academic Institution: University of Pittsburgh		**Major:** Microbiology	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, Nanoscale Metrology Group		
NIST Research Advisor:	Darwin Reyes-Hernandez		
Title of Talk:	Developing a Method for Measuring Intracellular Calcium Concentrations		

Abstract:

Diabetic patients frequently suffer from bone density loss, especially in the jaw bone. Osteocytes, bone cells that are embedded in the bone tissue matrix, regulate bone formation and resorption through a calcium signaling pathway triggered by a mechanical stimulus. If osteocytes signal for bone resorption, a different bone cell, osteoclasts, will break down the bone and release calcium ions to the bloodstream. We are using a microfluidic platform developed in our lab that allows us to position cells in close proximity (approximately eleven microns apart) to create a model of jaw bone tissue to study how changes in tissue environment affect the osteocytes and therefore the bone density. In order to determine how calcium concentration changes in osteocytes under stimulus, we needed to develop a method to measure intracellular calcium. Two fluorescent dyes that bind to intracellular calcium, Fluo-4 and Fura Red, were used with human aortic smooth muscle cells (HAoSMCs) to visualize and quantify changes in intracellular calcium before and after stimulation with tumor necrosis factor alpha (TNFα), a protein linked to inflammatory responses. Fluorescence was observed and recorded with a confocal microscope and analyzed using Fiji. The method developed can be applied to osteocytes in a bone jaw model in order to observe and understand the mechanisms by which osteocytes trigger bone formation and resorption.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Alana Dee		**Award Number**	70NANB18H132
Academic Institution: University of Pittsburgh		**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Pursuing a career in electrical engineering		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory (PML) Quantum Measurement Division Fundamental Electrical Measurements Group		
NIST Research Advisor:	Dean Jarrett		
Title of Talk:	Comparison of Current Detection Methods in the 3rd Generation Dual Source Bridge for DC Resistance Measurements		

Abstract:

The Metrology of the Ohm project is responsible for maintaining the resistance standards from micro-ohms to tera-ohms. Transfer standards and dual source bridges are used for these high resistance calibrations (1 MΩ to 100 TΩ). The third-generation dual source bridge balances to a true null, rather than a null offset as in the earlier NIST dual source bridges. This is based on the measured current across the bridge detector which requires accurate measurement of low currents in the pA range. The focus of this project has been to compare the performance of the existing current detector with the performance of a current-to-voltage conversion method. The latter detection method introduces a transimpedance amplifier, which converts currents in the µA, nA, and pA ranges to a voltage output detected by a high precision multimeter. The magnitude of the voltage output is a function of the gain setting on the amplifier. To determine the optimal gain setting for the amplifier, linearity tests are run by varying the gain, input current, and bandwidth. Additionally, a LabView user interface for the instruments was created to automate the data collection process. After confirming the linearity of the amplifier, it is added as a current detection option to the dual source bridge. The bridge, which measures a well-known 100 GΩ standard resistor, is run for each current detection method. The measured corrections are compared to the predicted correction of the 100 GΩ standard resistor. Based on the results, the more accurate current detection method will be implemented into the dual source bridge with the goal of reducing measurement uncertainty and increasing the efficiency of the calibration process.

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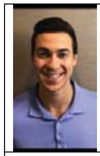
NIST – Gaithersburg, MD

August 7-9, 2018

Name: Michael Doris		**Award Number**	70NANB18H124
Academic Institution: California State University, Chico		**Major:** Physics, Electrical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursue a Master's Degree in Engineering and a PhD in Physics. Participate in research and development of renewable and/or nuclear energy, and transmission.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Laser Cooling and Trapping Group		
NIST Research Advisor:	Dr. Ian B. Spielman		
Title of Talk:	Encoding Arbitrary Phase and Amplitude Modes on Laser Light with A Digital Micro-Mirror Device		

Abstract:

Controlling the amplitude and phase structure of laser light is important for many applications in atomic, molecular, and optical physics where the ability to configure light has vastly improved probing and tailoring interactions between light and matter. The introduction of the liquid crystal spatial light modulator (LC-SLM, or SLM) and the digital micro-mirror Device (DMD) have enabled programmable control of laser light in applications such as optical tweezers, trapping, and imaging. The DMD is a faster alternative to the LC-SLM that can configure the amplitude and phase structure of light at rates upwards of 4kHz via millions of binary controlled micro-mirrors. Commercially available DMDs, commonly used by projector systems, are an economical and robust tool for crafting laser light in the lab. We demonstrate the DMD's ability to encode an arbitrary phase and amplitude mode on a laser beam via diffraction patterns, produce flat top probe beams, and generate a known reference for holographic imaging of cold atoms. Due to the programmable nature of the DMD, the beams engineered by these devices will improve the existing absorption imaging of atom clouds through real time stabilization of probe beam shaping, alignment, and positioning.



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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Benjamin P Eckardt	**Award Number** 70NANB18H126
Academic Institution: Bates College	**Major:** Mathematics & Physics
Academic Standing (Sept. '18):	Senior
Future Plans (School/Career):	Graduate School
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement, Laser Cooling and Trapping
NIST Research Advisor:	Ian Spielman
Title of Talk:	Increasing Efficiency of Temperature Controllers in the Laboratory

Abstract:
A Bose-Einstein condensate is a state of matter in which a macroscopic number of particles are made to occupy the same quantum state once cooled below a critical temperature. Bose-Einstein condensates extend the appearance of quantum phenomena to a macroscopic scale. They have been used to demonstrate properties such as superfluidity and superconductivity. In our lab, Bose-Einstein condensates of dilute gases of rubidium 87 are created through various cooling techniques in sequence. Rubidium, a solid at room temperature, needs to be vaporized in an oven at an elevated temperature, so that it can enter a Zeeman slower, where atoms are decelerated and precooled. For the stable operation of the oven, PID temperature controllers are used to keep the rubidium metal at target temperatures. The goal of this project is to implement the controllers such that they can be operated remotely, in order to bypass the extended wait time associated with warming up and stabilization. This talk will examine the scientific theory concerning the hardware utilization, the software implementation and general challenges faced.

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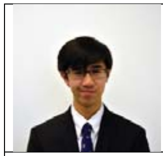
August 7-9, 2018

Name: Matthew Fu	**Award Number** 70NANB18H068
Academic Institution: Cornell University	**Major:** Engineering Physics
Academic Standing (Sept. '18):	Junior
Future Plans (School/Career):	Graduate School and a job doing research in industry or academia
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Semiconductor and Dimensional Metrology Division, Group 683
NIST Research Advisor:	Joe Kopanski
Title of Talk:	A Virtual Kelvin Probe Microscope

Abstract:
Kelvin probe force microscopy (KPFM) provides an accurate way of measuring the contact potential difference (CPD) between the tip and the sample and in extension the local work function of the sample. However, because the sample interacts with the entire probe, not just the tip apex, measurements from KPFM are dependent on the tip shapes. Through the usage of the physics modelling tool COMSOL Multiphysics, we have been able to model the different profiles of various tips, the geometry of the KPFM cantilever and sample setup, and the electrostatic and mechanical boundary conditions of the system to determine the dependence of the KPFM measurement on tip shape. We use two different physical models to conduct our simulations: one model uses the electromechanics interface in COMSOL to simulate the KPFM's mechanical vibration in response to the sample's CPD and the other uses the electrostatic interface in COMSOL to receive the potential reading from the sample. In this report, we will discuss the working principles of KPFM, and the effect of the tip shape on the systemic error in measurement collected by KPFM in both models. In addition, we will analyze the implications of such results in reconstructing the surface from the imperfect KPFM scan and the applications of this study including tip profiling and electric gradient measurement.



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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Kevin Ho		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate school		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Applied Electrical Metrology Group		
NIST Research Advisor:	Gerald FitzPatrick, Kang Lee, Eugene Song		
Title of Talk:	Development of Microgrid Simulation System for Hardware-in-the-Loop Study of Power Grid Monitoring and Control		

Abstract:
A microgrid is a group of interconnected loads and distributed energy resources that can "island" itself from the main utility grid and can operate independently by providing enough power to its loads. It strengthens grid resilience by helping to mitigate grid disturbances and by keeping high-quality power on for its customers. Today, microgrids have been developed to power hospital complexes, university campuses, remote island communities, and more.

Traditionally, devices used to measure voltages, currents, and power and to control the electric grid were analog devices. Analog voltage and current transformers scale high voltages and currents to usable levels, and they are pervasive in substations in today's grid. Recently, merging units (MUs) have been employed in power systems that convert analog current and voltage measurements into digital format as IEC 61850-9-2 Sampled Value (SV) messages. Based on the IEC 61850-9-2 standard, SV messages can be published via Ethernet LAN to protection devices, such as controllers or relays, to protect the grid more effectively. We intend to study interoperability and performance issues and requirements of various MUs.

For our study, we have developed a MATLAB/Simulink model of a microgrid, which uses photovoltaics, wind turbines, battery storage, and a diesel generator to power typical loads from a residential community and a small factory. An interface between the model and an OPAL-RT real time digital simulator provides the framework for a hardware-in-the-loop experiment of MUs. The OPAL-RT device will be used to provide three-phase ac current and voltage measurements from the simulation to MUs under study. The interoperability and measurement accuracy of MUs will be examined through comparison with calibrated reference digitizers. From these results we intend not only to present the strengths of MUs as essential components for monitoring, protection, and control of a microgrid, but also to determine where and what improvements are needed.

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August 7-9, 2018

Name: Wiley Hundertmark		**Award Number**	70NANB18H120
Academic Institution: Boston University		**Major:** BA: Earth and Environmental Sciences, MA: Remote Sensing and GIS	
Academic Standing (Sept. '18):	Undergraduate Junior; First-year Graduate Student		
Future Plans (School/Career):	Graduate school and a career in geospatial technologies		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science Division, Remote Sensing Group		
NIST Research Advisor:	David W. Allen, Ph.D.		
Title of Talk:	Using Optical Methods to Investigate Productivity and Carbon Fluxes in Urban Forests		

Abstract:
As the world's forests become progressively fragmented due to deforestation and development, it becomes increasingly important to study forest edges in urban environments because they behave differently than intact forests. The NIST campus offers an ideal testbed for such study, as it contains a fragmented temperate forest in a suburban area. To assess the characteristics of an 100m x 100m forested area, various sensors have been laid out across the plot to examine relationships between spatial position and temperature, respiration, and productivity. Measurements of soil and stem respiration, tree growth, soil moisture, sap flux, temperature, and evapotranspiration are taken on a minute-to-minute, daily, or weekly basis. Larger scale data are recorded using hyperspectral imagers, phenological and thermal infrared cameras, and pulse amplitude modulated (PAM) chlorophyll fluorometers. These optical sensors are used to support research into the field of Solar Induced Fluorescence (SIF), a developing technology using spectrometers to assess photosynthesis rates. When combined with other optical sensors, SIF may allow us to scale carbon fluxes up to regional and global scales.

Creating carbon balances of certain ecosystems is important because it allows us to establish more accurate estimates of terrestrial ecosystems' assimilation and response to climate change. This summer, a system was implemented designed to quantify the amount of carbon removed from the atmosphere by grasses bordering the forested plot. By combining CO_2 sensors with wind direction data, the flux of carbon dioxide between the vegetation and the atmosphere can be calculated. Furthermore, different iterations of the experiment will be performed to assess the extent to which certain changes to the vegetation - such as mowing or dark-adapting the grass - result in different fluxes of carbon.

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August 7-9, 2018

Name: Dylan Kirsch		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Materials Science and Engineering	
Academic Standing (Sept. '18):	1st Year Graduate Student		
Future Plans (School/Career):	Ph.D in Materials Science and Engineering		
NIST Laboratory, Division, and Group:	Physical Measurement Lab, Semiconductor and Dimensional Metrology Division, Nanoelectronics Group		
NIST Research Advisor:	Dr. Angela Hight Walker		
Title of Talk:	Raman Spectroscopy of Tin-based Intermetallic Thin-Film Libraries for Next Generation Rechargeable Battery Anodes		

Abstract:
As traditional energy resources continue to be depleted, studies on materials and devices aimed at advanced energy storage and conversion applications are on the forefront of many research efforts. More specifically, rechargeable (secondary) batteries hold great promise in many emerging areas that require power over extended distances or time. Since their commercialization in the 1990's, lithium-ion batteries (LIBs) have continued to receive attention with the aim of increasing the capacities of the cathode and anode materials beyond what has been reached with traditional commercial materials (i.e. graphite, lithium cobalt oxide). Specifically, anode materials that undergo an alloying reaction with lithium (Li), including silicon (Si) and tin (Sn), have been the primary focus of many research groups. These materials incorporate up to 4.4 Li-ions per atom, thus increasing the capacity significantly over that of graphite, which intercalates one Li-ion for every six carbon atoms. The issue, however, is that the lithiation of Si and Sn leads to a volume expansion of over 300%, resulting in the pulverization of the electrode and ultimately the failure of the battery. Work to mitigate this volume expansion issue has led to numerous publications, but material systems composed of two-element intermetallics based on Si or Sn show noteworthy promise. The main purpose of the additional non-active, metallic component in the intermetallic system is to create a structurally sound "lattice" within the material, which does not incorporate or uptake Li, and constrains the active material (Sn, Si) as it is lithiated. Herein, the structure and lithiation capacity of a co-sputtered Sn-based intermetallic thin film library of varying compositions, both before and after lithiation, are investigated using resonant Raman spectroscopy. Detailed analysis of the vibrational modes before and after the addition of lithium give insight into the lithium uptake, volume expansion, and phase distribution within the film. Raman spectroscopy proves to be a facile, noninvasive method for looking at the local bonding, structure, and disorder in samples. Optical microscopy is also used to gain insight on the heterogeneity of the materials both before and after lithiation, and is then correlated with the results from Raman spectroscopy. This work is in collaboration with the University of Maryland, in which other characterization techniques are being used to study the same system. This project will help determine the viability of these materials to provide volume expansion mitigation for the fabrication and realization of the next generation of LIBs.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Merrik Malin		**Award Number**	70NANB18H069
Academic Institution: West Virginia Wesleyan College		**Major:** Applied Physics	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	I plan on going to the University of Virginia to get my masters in Electrical Engineering		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Quantum Optics Group		
NIST Research Advisor:	Dr. Joshua Bienfang		
Title of Talk:	High Speed Control Circuit for Single Photon Avalanche Detection		

Abstract:
Single-photon avalanche diodes (SPADs) are a useful and convenient solid-state method to detect single photons. SPADs require control circuitry for their operation. This circuitry includes temperature control to cool the diode to a low-noise state, as well as circuitry to quench single-photon-induced avalanches and then reset the diode to its active state. We first built a compact temperature controller that monitors and controls the temperature inside the SPAD to at least -20 oC. Towards designing an active quenching circuit (AQC) we tested a variety of high-voltage high-speed transistors. In a SPAD-based detector the AQC must end the avalanche current flow by quickly reducing the voltage bias across that SPAD (by 20 V or more), holding it low for some time, and then returning it to its original bias to reset, or re-arm, the detector. Our testing of different transistors focused on speed and other properties that are not obvious in the datasheet (DS), to see which transistors were best suited for fast operation at the required voltages. Nine different transistors were tested to see which one could react the fastest and have the least amount of ringing, which determines how quickly the detector can be reset and re-armed. To raise the voltage, we tested positive metal oxide semiconductor field effect transistors (pMOSFETs) and to lower the voltage we tested a negative metal oxide semiconductor field effect transistors (nMOSFET). We found that the larger the reverse transfer capacitance (CRSS), the greater the ringing, which delays the re-arming of the detector. We also noticed that the smaller the input capacitance (CISS), the faster the transistor reacted to a drive pulse. This study of available MOSFETs will be useful in designing an active quenching and reset circuit for SPADs. Similarly, our design of a compact temperature controller is critical to the development of an overall SPAD detection system.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Laurelia R. May-Pohlman		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Career in Signal Processing and Communications		
NIST Laboratory, Division, and Group:	Physical Measurements Laboratory, Quantum Optics, Atomic Spectroscopy		
NIST Research Advisor:	Gillian Nave		
Title of Talk:	An Improved Reference for Spectrograph Calibration at Low-to-Moderate Resolutions		

Abstract:

Every element in the universe emits light of specific wavelengths, thus each has a unique emission spectrum. Astronomers use a variety of instruments, from satellites to telescopes, to collect and analyze the emission spectra of distant objects, and identify which elements form them. These instruments must be, by comparing the collected data to the reference spectrum of an element or set of elements. Thorium hollow-cathode lamps are currently used as the standard for high resolution spectrographs, and NIST researchers have created a working reference database using the thorium spectrum. However, this spectrum is too dense to use for calibrating low resolution spectrographs. Also, the spectra of other elements are known for the UV and visible regions, but not for the IR region.

The goal of this project is to expand the existing database to include the spectra of up to 5 additional elements, primarily over the IR and visible regions. Pen-ray lamps are a good substitute for hollow-cathode lamps, since they are available for a variety of elements, they do not require high level current, they are easy to use and are already in use on astronomical spectrographs. This database differs from the NIST Atomic Spectra Database (ASD) in that it includes a visual plot of the spectrum, which is a more user-friendly standard for evaluating experimental data. The elements to be included are neon, argon, xenon, as well as mercury-argon and mercury-xenon combinations; each lamp is tested for three different currents. Using a 2-meter IR/visible/UV Fourier Transform Spectrometer (FTS), the intensity of emitted light is recorded as a function of wavelengths ranging from 300nm to 9000nm approximately; each element has a unique spectrum of intensity peaks, or lines. These spectra are calibrated using a separate light source, in our case a Tungsten lamp, as an intensity standard. The recorded spectra will then be added to the existing thorium database, as well as a table listing all available information about the spectra, namely, line positions, intensities, and uncertainties. Ultimately, this should provide a more complete reference for calibrating astronomers' and other scientists' instruments.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: James McLaurin		**Award Number**	70NANB18H119
Academic Institution: University of the District of Columbia		**Major:** Mechanical Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursuing graduate school – Mechanical Engineering		
NIST Laboratory, Division, and Group:	Physical measurement laboratory, Division 683, Nanoscale Metrology Group		
NIST Research Advisor:	Andras Vladar and Kate Klein		
Title of Talk:	Investigation of substrate suitability for focused helium ion beam machined nanofluidic structures		

Abstract:

The Orion helium ion microscope (HIM) is known for its sub nanometer imaging capabilities like a scanning electron microscope (SEM). Since helium does have a non-negligible mass it has limitations when it comes to imaging dose, but possesses promising capabilities for machining. Helium interacts differently with substrates that may be classified into two categories based on their structural properties: those that mill and those that deform. In this study we will create a table of materials and their properties to predict which regime they will fall under.

Most notably, when a helium ion beam is applied at high doses (>10^17 ions/cm^2) to a silicon substrate the sputtering (removal) rates of silicon are surpassed by implantation rates, which induces swelling deformation just below the substrate surface. This swelling causes bubbles to form, coalesce, and create pipe-like structures with controlled dose patterning. This novel method can rapidly produce complex nanofluidic structures that may have previously been too tedious or difficult to prototype. With the gallium focused ion beam (FIB), we will cross section the fluidic structures. This enables characterization of their fluidic capacity and functionality. This work may be especially important to assist in the acceleration of diagnostics new application discovery, and standards related to lab-on-a-chip microfluidics.

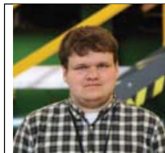
SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Stephen Meek		**Award Number**	70NANB18H099
Academic Institution: Montgomery College		**Major:** Biotechnology	
Academic Standing(Sept.'18):	Senior @ Montgomery College		
Future Plans (School/Career):	Augmenting current biotechnology studies with prior electronic engineering experience to participate in the development of improved instrumentation for biotech applications		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science Division, Fluid Metrology Group		
NIST Research Advisor:	Dr. Greg Cooksey		
Title of Talk:	An improved method to measure very low fluid flow rates for diagnostic medical and biotechnology applications		

Abstract:
This presentation describes an improved method for accurately measuring very low fluid flow rates on the order of tens of nanoliters per minute. In contrast to existing flowmeters, which are expensive and typically cannot make rapid measurements with high accuracy, we utilized microfluidic devices with integrated optical waveguides to deliver excitation light and collect emitted light from fluorescent materials in flow in real time. We demonstrate fluid flow measurements with a solution containing fluorescein, a fluorescent dye that can be used to visualize flow in a microchannel. When stimulated with 488nm light, fluorescein emits 520 nm light. Critically, for our measurement process, fluorescein is also destroyed when the molecules receive a high dosage of light (either due to high excitation power or slow velocity through the excitation beam). Due to the no-slip boundary condition of pressure driven flow in this device, a parabolic velocity profile is created across the channel: molecules on the edge of the channel have zero velocity and receive the highest dosage, while molecules at the center of the channel move the fastest and receive the lowest dosage. We explored the scaling relationship across different dosages by measuring fluorescence efficiency across a range of excitation powers and flow rates. Namely, the excitation laser was stepped from 0 to 60 mW in 10% increments for each flow rate tested between 10 nl/min to 5000 nl/min. As dosage increased, either due to increased laser power or decreased flow rate, more fluorescein molecules are photobleached, resulting in a decreased fluorescence efficiency. The results indicate that even with only order-of-magnitude estimates of the device geometry and operating conditions, the scaling relationship holds to within 10% relative uncertainty over 3 orders of magnitude. Overall, the optofluidic method presents new opportunities to continuously measure very low flow rates with low uncertainty. We find the device is incredibly sensitive to changes in flow very near 0 nl/min, but overall the accuracy of the measurement is limited by the accuracy of a commercial flow meter, which has an absolute uncertainty of about 100 nl/min. Techniques to validate flow measurements below 100 nl/min are being evaluated.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: David Andrew Mullins		**Award Number**	70NANB18H136
Academic Institution: University of Kentucky		**Major:** Physics	
Academic Standing (Sept. '18):	Fulbright Scholar		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Radiation Physics, Neutron Physics		
NIST Research Advisor:	Daniel Hussey		
Title of Talk:	Neutron Bragg Edge 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, a technique known as Bragg-Edge imaging was used to determine the composition of a sample meteorite. By imaging the sample with multiple wavelengths of neutrons, the neutron attenuation as a function of wavelength can be determined. Using Bragg's Law, this change in neutron attenuation can be used to determine the lattice spacing within the sample. By collecting tomographic reconstruction data at each wavelength, the lattice spacing can be determined for each voxel within the sample. Matching the lattice spacing to a material creates a 3D map of the materials contained within the meteorite.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Vaishnavi Murthy		**Grant Number**	70NANB18H153
Academic Institution:	University of Maryland, College Park	**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Graduate Studies		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Mass and Force Group		
NIST Research Advisor:	Corey Stambaugh		
Title of Talk:	Environmental Monitoring and Control for Metrological Applications		

Abstract:

Beginning in 2019, NIST will disseminate the unit of mass from two ensembles of mass artifacts: One ensemble will be maintained in air at atmospheric conditions, while the other will be maintained under vacuum at a pressure of approximately 10^{-3} Pa. For the ensemble stored in air, it is important that the pressure, temperature, and relative humidity are controlled within certain limits to ensure stability of the mass artifacts. Last year I developed a microcontroller-based humidity control system that uses the "bubbler method" to maintain the relative humidity inside a storage chamber since the long-term variation of humidity may be responsible for significant mass changes for stainless-steel artifacts

This year I am studying the feasibility of using various low-cost humidity, pressure, and temperature sensors as an accurate, low-cost environmental monitoring system. These sensors combined with the previously mentioned humidity controller will be compared against calibrated environmental sensors. To acquire and log environmental data, I have developed software that utilizes a user-programmable FPGA in conjunction with the LabVIEW programming environment. By collecting humidity, temperature, and pressure data from chip-based devices over long periods (weeks) and short periods (days), we can determine the suitability of low-cost IC sensors for use in precision metrology applications.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Peter Orban		**Award Number**	70NANB18H108
Academic Institution:	St. Mary's College of Maryland	**Major:** Mathematics and Physics	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Radiation Physics Division, Radioactivity Group		
NIST Research Advisor:	Denis Bergeron		
Title of Talk:	Ionization Chamber Response Dependence on Ambient Environmental Conditions		

Abstract:

Reentrant ionization chambers (ICs) are commonly used for high-precision radioactivity measurements. Recently, some researchers have interpreted seasonal variations in chamber responses as evidence for non-constancy of radioactive decay constants. These researchers have attributed variation in decay constants to the Earth's orbit around the sun, citing the dependence of solar neutrino flux on Earth-Sun distance as impacting radioactive decay rates. However, ICs are also known to be sensitive to changes in ambient conditions such as temperature, pressure, and relative humidity—quantities that, like solar neutrino flux, exhibit seasonal variations. Before a new theory about changing decay constants can be considered, we first must better understand the effects of environmental conditions on IC responses.

Using a weather station from Extech Instruments, we obtained temperature, pressure, and relative humidity data. We used a Ra-226 source to measure IC responses, mainly from a Capintec Radioisotope Calibrator (CRC-15R) and a Vinten 671 Ionization Chamber (VIC). A Ra-226 source is effective for constancy checks due to its long half-life of 1600 years. Therefore, only a negligible change in activity occurred over the course of this experiment. Over a short sampling period this summer, we have seen signs of correlation, especially between relative humidity and IC readings thanks to a chilled water outage. Additionally, we developed tools in LabView to match the environmental data with the IC data based on timestamps. Furthermore, we are working on creating tools in LabView so the weather data can automatically be incorporated with the regular IC data program.

Environmental conditions, particularly relative humidity, appear to be correlated with changes in IC response. More research must be conducted to better understand the effects of environmental conditions on IC responses. It is essential that we understand these effects so we can correct for them before searching our data for signs of new physics.

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NIST – Gaithersburg, MD

August 7-9, 2018

Name: Sumaiyah Sarwat		**Award Number**	70NANB18H153
Academic Institution: University of Maryland, College Park		**Major:** Electrical Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Preferably work in the industry before pursuing a Master's Degree or a PhD.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement, Applied Electrical Metrology		
NIST Research Advisor:	Richard Steiner		
Title of Talk:	Watt-Hour Meter Testing		

Abstract:
In the past couple of years, there has been a transformation from traditional electric grids to smart grids in many parts of the world. A smart grid is an electrical grid which includes a variety of operational and energy measures including smart meters, smart appliances, renewable as well as energy efficient resources. It allows a two-way flow of electricity and information that is capable of monitoring power plants, customer preferences, and individual appliances/equipment.

One of the most important devices used in a smart grid is a smart meter. The smart meter is an advanced energy meter that obtains information from the end users' load devices and measures the energy consumption and provides additional information to the utility company for better monitoring and billing. The smart watt-hour meters have proven to be more reliable than the traditional electromechanical watt-hour meters. However, the smart meters may still be vulnerable to inaccuracies when subjected to non-sinusoidal waves, loads with a high order of harmonics resulting in distorted power signals.

We worked on software that tests 8 smart meters, under sinusoidal and non-sinusoidal (distorted) power using dimmers, standard light bulbs, and LEDs. My part in the project was to plot results relative to various distortion levels and develop a program in LabVIEW that is used to calculates the harmonics of the test waveform. The test results of the changes in the smart watt-hour meter accuracy are compared to the analyses of the harmonics produced by the distorted waveforms.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Jacob Siegel		**Award Number**	70NANB18H153
Academic Institution: University of Maryland College Park		**Major:** Physics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Physics Graduate School		
NIST Laboratory, Division, and Group:	PML, Sensor Science Division, Thermodynamic Metrology Group		
NIST Research Advisor:	Stephen Eckel		
Title of Talk:	Constructing a Primary Vacuum Standard using Bitter Electromagnets		

Abstract:
Current vacuum gauges operating in the ultra-high-vacuum (UHV) and extreme-high-vacuum (XHV) regime are not primary and have poorly understood uncertainties. We are creating a UHV and XHV primary standard. To make the primary standard, laser cooled lithium atoms are stored in an Ioffe-Pritchard magnetic trap, where they can be ejected by background gas collisions. By measuring the ejection rate we can obtain the background gas pressure. At XHV pressures, atoms are ejected over a time scale of one hour. To ensure the magnetic fields remain constant over one hour we built a Bitter-type electromagnet. The Bitter electromagnet is a stack of copper and insulating Teflon, creating an electromagnet where cooling water flows parallel to the electric current. The 435 parallel cooling channels allow for high heat dissipation and an even temperature across the magnet, leading to a stable field over time. We characterize the magnet by measuring the temperature rise for a given current flow, coil inductance, current noise and the turn on time of the Bitter electromagnet.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 7-9, 2018

Name: Alexander J. Sredenschek	**Award Number** 70NANB18H097
Academic Institution: Messiah College	**Major:** Physics and Mathematics
Academic Standing (Sept. '18):	Senior
Future Plans (School/Career):	I plan to pursue a Ph.D in physics after I graduate to prepare for a career in research and education as a physics professor.
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Division 683, Group
NIST Research Advisor:	Dr. Christina Hacker
Title of Talk:	Silicon Surface Functionalization for Battery Applications

Abstract:
Lithium-ion batteries are widely used in our everyday lives, found in items such as power tools, cellphones, and computers. They are efficient, easy to manufacture, and rechargeable. However, the current materials used in these batteries do not provide competitive energy output for larger devices, such as electric cars and industrial tools. Researchers have focused their attention on replacing the current anode material—graphite—with silicon. Silicon has a theoretical energy density that is ten times higher than that of graphite, but upon electrochemical cycling, silicon undergoes significant volume expansion (roughly 400%), yielding electrode damage and reduced battery performance. The key to resolving this issue is understanding the interface between the anode and the electrolyte, a film called the solid electrolyte interphase (SEI). Much work has been done on investigating the effects of novel electrolyte solutions and anode structures (silicon nanoparticles, Si-C mixtures, nanowires, etc.) on SEI evolution. One technique that has not yet been studied is coating silicon with monolayers.

In this research, we attach alkane monolayers to n-type silicon with Si-S-C and Si-O-C bonds via mono/disulfides, alcohols, and acids. Monolayers are terminated with carbonyl and methyl groups to elucidate the nature of the SEI. Our samples are characterized ex situ using Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), spectroscopic ellipsometry (SE), and scanning electron microscopy (SEM) before and after electrochemical cycling using cyclic voltammetry (CV). Upon two lithiation/delithiation cycles, samples show an increase in film thickness and lithium content. We also investigate the effects of monolayer structure on the evolution of SEI components.

SURF Student Colloquium
NIST – Gaithersburg, MD
August 7-9, 2018

Name: Eileen Stauffer	**Award Number** 70NANB18H153
Academic Institution: University of Maryland, College Park	**Major:** Physics
Academic Standing (Sept. '18):	Junior
Future Plans (School/Career):	Pursuing career in applied physics
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science Division, Thermodynamic Metrology Group
NIST Research Advisor:	Zeeshan Ahmed
Title of Talk:	Evaluation of FPGA-Based Laser Stabilization

Abstract:
Photonic sensors use properties of light, such as frequency, to make high precision measurements of parameters such as temperature and humidity. These measurements often require the use of laser locking, a technique in which a control loop is used to lock the laser frequency an optical sensor. A field-programmable gate array (FGPA) can be used to replace elements of an analog laser lock system and thus cost-effectively reduce the system footprint. We implement a FPGA based laser lock on temperature and humidity sensors and evaluated the results against those obtained using traditional analog lock.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Alexander S. Todd	**Award Number** 70NANB18H121
Academic Institution: Indiana University	**Major:** Physics
Academic Standing (Sept. '18):	Junior
Future Plans (School/Career):	Pursuing a career in Applied Physics
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Radiation Physics, Neutron Physics
NIST Research Advisor:	Daniel Hussey
Title of Talk:	Far Field Neutron Interferometry

Abstract:
Experiments relating to non-destructive imaging and subsequent three-dimensional reconstructions have traditionally been performed using x-rays. However, because x-ray absorption scales directly with sample density, x-rays are not optimal for imaging objects with higher densities. Neutrons can more effectively image denser materials by slightly modified methods originally intended for x-rays because neutron scattering cross sections vary proportionally to the strong nuclear force instead of sample density.

The wave-like properties of neutrons allow the effective function of a far-field interferometer, from which dark-field images can be collected and analyzed. When manipulated with several precisely aligned diffraction gratings, neutrons can then be used to create a moiré pattern, which improves the quality of data collected by the detector. As the neutron beam passes through samples, it is de-phased and a smaller visibility is recorded by the camera. This allows the detection of microstructures within a sample, and when many such projections are collected at different angles with respect to the neutron beam, tomographic methods can be used to recreate a three-dimensional scattering pattern of the sample. This can be further analyzed to understand the type of materials the sample consists of, as well as their organization.

Specifically, this method of neutron imaging was used to analyze several samples, such as Westerly granite, at optimized parameters. At an instrument length of 3.5-meters, neutron wavelengths of 4-Angstroms, and source gratings of 200, 600, and 1200 microns, visibilities on the order of 0.1 were detected.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Hunter Wages	**Award Number** 70NANB18H123
Academic Institution: Wofford College	**Major:** Physics and Applied Mathematics
Academic Standing (Sept. '18):	Senior
Future Plans (School/Career):	Planning on going to grad school for either Math or Physics
NIST Laboratory, Division, and Group:	Physical Measurement Lab, Sensor Science Division, Remote Sensing Group
NIST Research Advisor:	Dr. Solomon I Woods
Title of Talk:	Using Magnetic Field Inversion to Produce Current Density and Magnetization Distribution Images

Abstract:
Currently, there is no non-invasive method of creating a 3-dimensional image of the temperature distribution throughout a volume. Using multi-layer magnetic nanoparticles that have magnetizations that are highly temperature dependent, we will possibly visualize temperature within a volume for the first time. By distributing these magnetic nanoparticles inside of a volume and measuring their resulting magnetization, we can calculate the temperature at a specific location within the volume. In previous studies, magnetic inversion techniques of the Biot-Savart Law have been used to create programs that determine current density distributions from the magnetic fields they create. To fully understand these computational techniques, we developed a program in MATLAB that performs this magnetic field inversion. Using that program as a guide, we programmed a very similar inversion technique on the Magnetic Dipole Field equation which, when given magnetic field data, can determine a magnetization distribution.

The quality of results from these programs are highly dependent on the scan height of the magnetic field sensor above the sample and the windowing function that is used to filter noise from the magnetic field. These programs utilize an error function that loops through a range of scan heights and windowing function sizes to optimize the scanning conditions for a given experimental configuration. These inversion programs have been tested using simulated data in COMSOL and have yielded accurate current density and magnetization distribution images. Since these programs have been tested and proven to produce accurate images, they are ready to image the magnetization distribution of these nanoparticles, which will allow us to depict temperature throughout a volume for the first time.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Francis Walz		**Award Number**	70NANB18H113
Academic Institution: Towson University		**Major:** Applied Physics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Attending graduate school for a degree in material physics		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Atomic Spectroscopy Group		
NIST Research Advisor:	Dr. Joseph Tan		
Title of Talk:	An active LCR circuit for cooling highly charged ions captured in an ion trap		

Abstract:

Precise spectral measurements in highly charged ions (HCI) are needed for potential new applications in high precision atomic clocks, quantum information processing, and the search for variations in the fine-structure constant. Highly ionized atoms are produced in an Electron Beam Ion Trap (EBIT) consisting of static magnetic and electric fields to confine ions and an integrated electron gun to create the ions. As a result of the electron bombardment, the ions acquire stellar temperatures, and hence precise spectral measurement is limited by Doppler effects. By extracting the ions from the EBIT and capturing/isolating them into an ion trap, the temperature can be lowered by two orders of magnitude. One way to further cool the extracted/stored ions is to dissipate their thermal motions in an external circuit. In this resistive cooling method, the trap electrodes are attached to a high-Q circuit which is driven by the induced currents from the confined ions that are being cooled. The induced current from the oscillating ions passes through a resistor and releases energy in the form of heat (joule heating). Our goal is to develop a resonator circuit with appropriate inductance, resistance, and capacitance (LRC) that will couple to the trapped ions with a high Q factor for efficient cooling. We will use an analog-simulated inductor using a gyrator circuit which includes 2 operational amplifiers (op-amps) because of its ability to adjust the Q factor and provide a wide range of inductance. Cooling the isolated highly-charged ions from 5 eV to near room temperature would improve spectroscopy, and open the possibility of direct laser cooling to much lower temperatures.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Galahad Wernsing		**Award Number**	70NANB18H065
Academic Institution: Worcester Polytechnic Institute		**Major:** Electrical & Computer Engineering	
Academic Standing (Sept. '18):	Graduate Student		
Future Plans (School/Career):	I am pursuing a masters degree in ECE at WPI. Long term I would like to end up in an industry research position.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Engineering Physics Division, Nanoelectronics Group		
NIST Research Advisor:	Jared Wahlstrand, Alan Bristow		
Title of Talk:	Real Time Data Analysis and Phase Correction for Optical 2D Spectroscopy		

Abstract:

Optical 2D spectroscopy is a powerful time-domain technique that uses short laser pulses to investigate electrodynamic properties of many types of material. The technique is relatively new and still under active development; data is collected using entirely custom-built systems. In the Nanoelectronics Group, optical 2D spectroscopy is achieved with three pulses from a Ti:Sapphire laser generating a four-wave-mixing signal, the amplitude and phase of which is measured by interference with a reference pulse. Complicated analysis is required to extract the data and even to tell if something went wrong during the data taking process.

This project developed sophisticated, dynamic and versatile data analysis code and implemented real time data processing alongside data acquisition. Real time processing provides the ability to detect data collection problems early which speeds up the debugging process, and the code structure supports a range of spectroscopic types associated with the order of optical pulses and polarization configuration.

Much of the power of 2D spectroscopy is its ability to capture both phase and amplitude information, which is achieved though phase stabilization or correction of a reference pulse. In previous experiments the phase drift was locked using an external system, but the lock did not perform well using the lower light intensity required for some samples. Using a second camera, we can measure the phase drift over the duration of the experiment and add a correction to the data during post-processing. This makes the data processing code more complicated but allows our experimental setup to study a wider range of sample materials.

In our experiment, we use results of optical 2D spectroscopy of a GaAs semiconductor microcavity, to test the new real time analysis code and user interface, both implemented in Python. Results of the analysis code are shown for multiple polarization configurations which allow for separation of different contributions to the optical response.

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NIST – Gaithersburg, MD
August 7-9, 2018

Name: Zach Whiting		**Award Number**	70NANB18H069
Academic Institution: West Virginia Wesleyan College		**Major:** Applied Physics	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Applying to graduate schools for Medical Physics.		
NIST Laboratory, Division, and Group:	Physical Measurements Laboratory, Radiation Physics Division, Dosimetry Group		
NIST Research Advisor:	Dr. Ronald Tosh		
Title of Talk:	Graphite Calorimetry with a Mach-Zehnder Interferometer		

Abstract:
Striving to improve cancer therapy, doctors and scientists alike are looking to discover new and better treatments. Wherever such treatments involve external-beam radiotherapy, successful outcomes require accurate determination of absorbed dose, or the measure of how much energy is deposited by the beam per unit mass of the target tumor. Primary standards for medical radiation dosimetry in the US are developed and maintained at the NIST, and the current primary-standard instrument is a water calorimeter that uses thermistors and lock-in detection to achieve microkelvin sensitivity. The instrument is designed to work with static, spatially uniform beams, whereas modern cancer therapy usually involves complex, time-variable beam profiles for which the current primary standard; hence any calibration based upon it is ill-fitted. To address this deficiency, the NIST radiation Dosimetry Group has been exploring methods of interferometer-based calorimetry that may enable time-resolved 3D dose profile reconstruction. The first objective is realizing the desired temperature sensitivity in a tissue-equivalent target material, of which water and graphite are typically used in radiation calorimetry. For this work, we have constructed a Mach-Zehnder interferometer with graphite posts and are characterizing both its mechanical stability and sensitivity to Joule heating input by measuring small (~0.001 radian) phase shifts in its interference pattern. Plans include studying its dose response in the NIST Medical Industrial Radiation Facility and the NIST Clinac 2100C medical linac.

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SCO/TPO

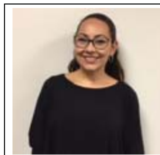
Last Name	First Name	Lab
Corrigan	Alexsandra	Special Programs
Guzman Cruz	Yinaris	Special Programs
Ionescu	Candice	Special Programs
Resto Garcia	Angel	Special Programs
Taylor	Zachary	Special Programs

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Alexsandra Corrigan		**Award Number**	70NANB18H109
Academic Institution: Virginia Tech		**Major:** Biochemistry and Biology	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Special Programs, Standards Coordination Office(SCO), Headquarters Materials Measurement Laboratory(MML), Biosystems and Biomaterials		
NIST Research Advisor:	Clare Allocca (SCO), Laura Pierce (MML), Sumona Sarkar (MML)		
Title of Talk:	A Cell-ing point for Standards: Terminology and Analytical Methods for Biotechnology Standards		

Abstract:
International standards are a critical component of commerce, including industry best practices, product measurement, and terminology use. The International Organization for Standardization (ISO) established Technical committee (TC) 276 to develop voluntary consensus standards for biotechnology to enable more reliable, higher quality and better understood globally competitive products. This project contributed to the advancement of TC276 standards via terminology exploration and analytical investigations into cell counting measurements.
To clarify terminology use within biobanking, contributions were made to a biobanking ontology. This ontology will help to define relevant terms and their relationships. Contributions were also made to documents helping to elucidate the work of TC276 as a whole, and the process of becoming involved in standards creation.
With the growing use of Cell Therapy Products (CTPs) there is an increased need to develop standardized methods for counting and characterizing cells, and assessing viability. There are difficulties in measuring cells due to variations in size, morphology, and stages of cell death. Many of the instruments that count cells are image-based and characterize viability based on image features. Differences in instrument settings can lead to variability in image quality, which impacts cell count and viability measurements.
To address these challenges, a design of experiments (DOE) is being conducted to determine optimal imaging settings for the Cellometer Auto 2000, and to determine which settings image analysis may be most sensitive to. We seek to optimize the performance of the instrument by establishing the appropriate settings to acquire high quality images for analysis. Preliminary experiments using polystyrene microsphere bead controls were used to capture images at a range of focus and brightness settings. In collaboration with Information Technology Laboratories(ITL), we have generated a blur metric from the beads which can correlate focus levels with image quality.
Further experiments will test the impact of additional parameters such as cell concentration, trypan blue concentration, and other cell conditions. With this experimental design, we seek to provide a valuable tool to aid biotechnology companies in assessing image quality in cell viability analyzers.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Yinaris Guzman Cruz		**Award Number**	70NANB18H127
Academic Institution: University of Puerto Rico Mayaguez		**Major:** Industrial Engineering	
Academic Standing (Sept. '18):	Junior		
Future Plans (School/Career):	Pursue a career as an Industrial Engineer		
NIST Laboratory, Division, and Group:	TPO, Division 401		
NIST Research Advisor:	Paul Zielinski		
Title of Talk:	Advanced Manufacturing and Development and growth of technology-based businesses in Puerto Rico		

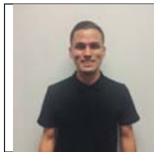
Abstract:
The Technology Partnership Office deals with the relationship between laboratories and NIST industries, it is the link for customers to find and learn about the new technology available. NIST seeks to facilitate connections between the industries of Puerto Rico and the more than 300 federal laboratories of 11 federal agencies to develop new technological opportunities. This intense research aims to create connections with the industries of Puerto Rico, improve the new technology on the island and therefore improve the quality of life of citizens. In addition, I worked with the NIST Advanced Manufacturing program by preparing data and summaries of the patents and licenses of the NIST inventions in this field. Thus, the industries could obtain a complete summary of the inventions and patents of NIST.
An analysis was made of the businesses and industries in Puerto Rico with relevant information to conduct business in the future. The companies were classified into industrial sectors using the North American Industry Classification System (NAICS) to allow connections between the products of each industry with possible laboratories that can help the business. We worked with the material for the NIST intellectual property license related to Advanced Manufacturing to establish connections with companies that will develop and use the technologies. In conclusion, information was obtained from more than 1000 companies and their respective classifications to establish the connections between the products or services and the laboratories.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Candice Ionescu		**Award Number**	70NANB18H156
Academic Institution: Dickinson College		**Major:** International Studies	
Academic Standing (Sept. '18):	Senior @ Dickinson College		
Future Plans (School/Career):	Fulbright ETA and Graduate School in International Trade/ Finance		
NIST Laboratory, Division, and Group:	Standards Coordination Office		
NIST Research Advisor:	Jennifer Marshall		
Title of Talk:	China's Changing Standards Infrastructure: A New Approach to the Global Stage		

Abstract:
China's approach to developing standards provides a unique contrast to the approach used by the United States. A compelling case study is the Wireless Local Area Networks Authenticity and Privacy Infrastructure (WAPI) standard vs. the Wireless Fidelity (WiFi) standard which highlights the technological and geopolitical differences between the US and China as presented on the global standards-setting stage. The unsuccessful attempt at garnering support to create the national WAPI standard into an international standard, caused the Chinese to increase their levels of ISO (International Organization for Standardization) technical committee participation and change their standardization infrastructure for more influence in international standardization organizations (SDOs). Countries want to influence standards development because of standards essential patents that generate significant revenue from the royalties received by licensing the technology required to comply with that standard. The WAPI vs. WiFi case is a perfect example of this, because after years of standardization law reform, the Chinese wanted their WAPI standard to become the internationally accepted ISO wireless local area networks standard, however, it was blocked by the US-backed WiFi standard that was developed by the Institute of Electrical and Electronics Engineers (IEEE) and globally adopted. China's actions in seeking to set its own WAPI standards, instead of adopting international standards, questioned their responsibility to reducing technical barriers to trade as a World Trade Organization Technical Barriers to Trade (TBT) Agreement signee. The Chinese realized that their state-run domestic approach to standardization was not applicable internationally and moved to develop more industry-run US infrastructure to standards development, while simultaneously increasing their ISO technical committee participation in convenorships and secretariats. By becoming strategic at the standards development, they are poised to challenge US dominance in setting standards that impact international trade.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 7-9, 2018

Name: Ángel Jarel Resto García		**Award Number**	70NANB18H128
Academic Institution: SUAGM-Universidad del Turabo		**Major:** Industrial & Management Engineering	
Academic Standing (Sept. '18):	Senior		
Future Plans (School/Career):	Pursuing a career in Industrial & Management Engineering		
NIST Laboratory, Division, and Group:	Technology Partnerships Office (TPO)		
NIST Research Advisor:	Paul Zielinski, Donald Archer		
Title of Talk:	Advanced Manufacturing & Development and growth of technology-based businesses in Puerto Rico		

Abstract:
The research fellowship internship with the Technology Partnerships Office (TPO) involves many projects and desired goals for this summer period. The two main areas of research focus on the field of Advanced Manufacturing and the development and growth of technology-based businesses in Puerto Rico. The Advanced Manufacturing task requires data analysis and summarizing activities in order to find industry partners to commercialize NIST patents through the licensing of the inventions created in the NIST labs. Many scientific disciplines are performed in these labs, such as additive manufacturing, biomanufacturing, lean manufacturing, machining, robotics, supply chain, quality assurance, process improvement, process measurement and more. The growth of technology-based businesses in Puerto Rico task involves the development of technology transfer areas for an industrial impact improvement on the island of Puerto Rico. This task starts with examining and defining the business ecosystem on the island to identify technology growth areas, explore and define targeted market opportunities. The second part of the task is to develop avenues to enhance communications between federal laboratory infrastructure and the business community for a future technology event development on the island.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 7-9, 2018

Name: Zachary Taylor		**Award Number**	70NANB18H083
Academic Institution: North Carolina State University		**Major:** Computer Science	
Academic Standing (Sept. '18):	Sophomore		
Future Plans (School/Career):	Pursuing a career in the computing industry.		
NIST Laboratory, Division, and Group:	Technology Partnerships Office, Division 401, Group 00		
NIST Research Advisor:	Paul Zielinski		
Title of Talk:	Technology Transfer, Invention Disclosures, and Supporting the MBDA Mission		

Abstract:

The field of technology transfer bridges the gap between research and industry by facilitating relationships between researchers and industry partners to effectively transfer new technologies and commercialize them. Mechanisms such as licensing and cooperative research and development agreements support these efforts. When licensing government-created technologies, technology summaries play an important role. Equipped with a basic knowledge of an invention in a lab and its potential impacts, industry partners can make informed decisions about which technologies are suitable to promote for further commercialization.

One dimension of technology transfer that often gets overlooked is the level of technology transfer to minority-owned businesses. Considering this, the DOC's Minority Business Development Agency (MBDA) supports minority-owned businesses by providing one-on-one assistance at MBDA centers throughout the country to help perform tasks such as writing business plans and marketing.

This summer, I worked in the Technology Partnerships Office at NIST, where I worked both internally on invention disclosures and externally with the MBDA. Internally, I wrote technology summaries for information technology-related invention disclosures that could be added to the "Available Technologies" section of the Federal Labs website. With the MBDA, I helped analyze data on minority-owned firms to better understand prominent high-tech industry groups in each state. During this analysis, I realized that the methods I was using could be automated, so I created an R script that would perform the analysis more quickly. Afterwards, I created an R Shiny web application that provides an intuitive user interface for the task.

My work will help further an understanding of industries in which minority businesses are engaged and will aid in the preparation of regional MBDA meetings throughout the country. My contributions in the form of technology summaries will enable a stronger relationship between researchers at NIST and potential industry partners who could commercialize their inventions.

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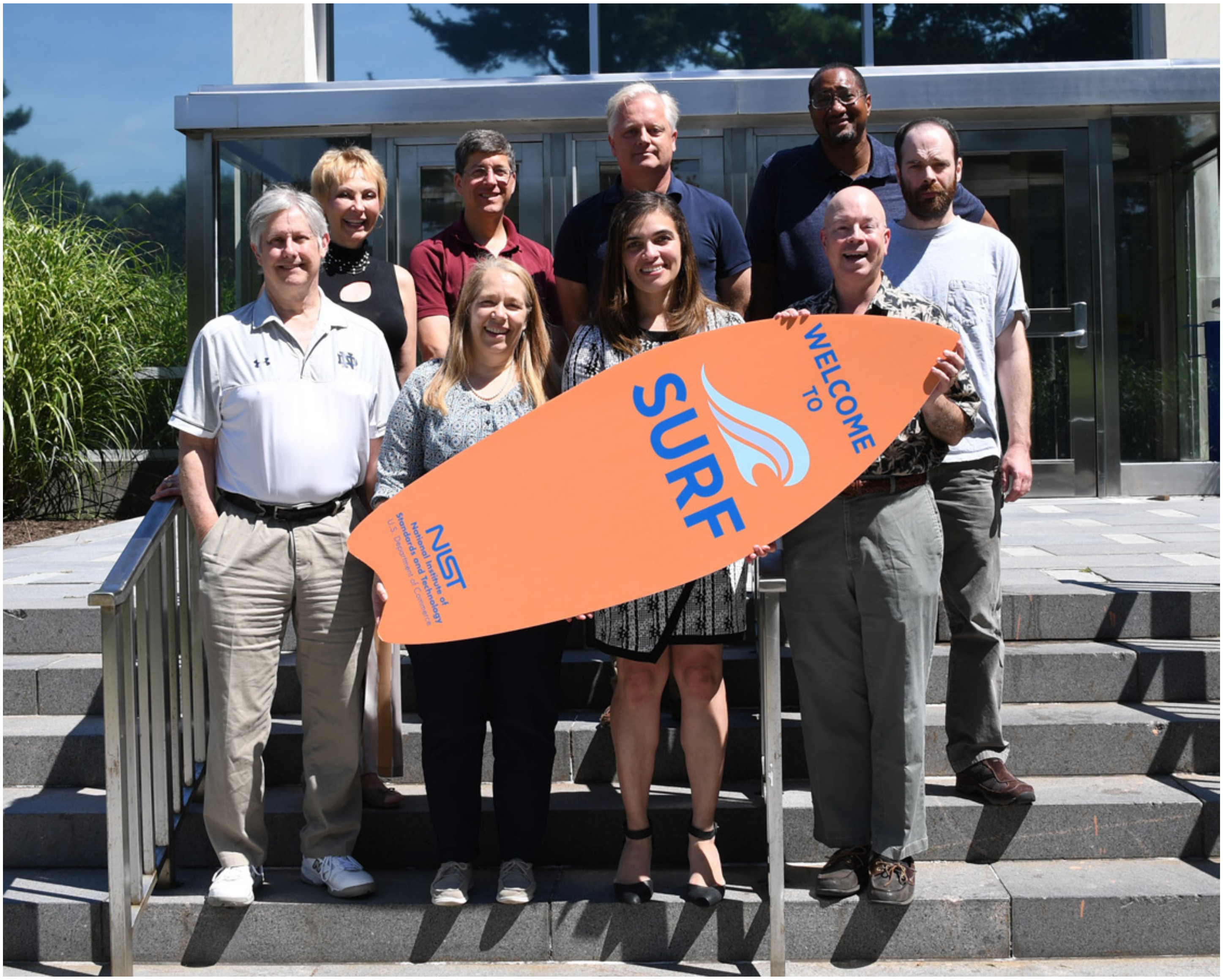


SURF Directors

T-Shirt Committee

Meal with a Mentor

SURF

Capitol Hill

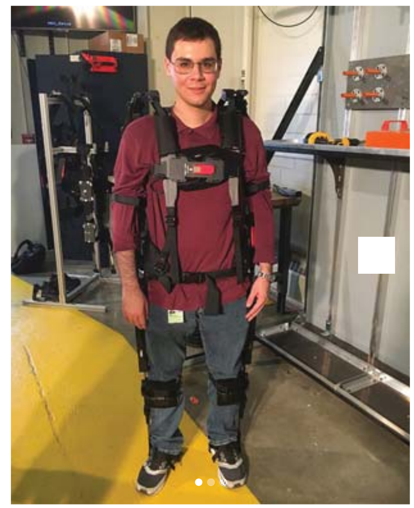
usnistgov • Following

usnistgov SURF NIST! More than 200 undergraduate students converged on the NIST Gaithersburg and Boulder campuses today for the start of the SURF (Summer Undergraduate Research Fellowship) program. The students will spend 11 weeks this summer contributing to ongoing research in a variety of disciplines. We look forward to sharing their stories and pictures throughout the summer.

Find out more about the SURF program at

190 views

MAY 29



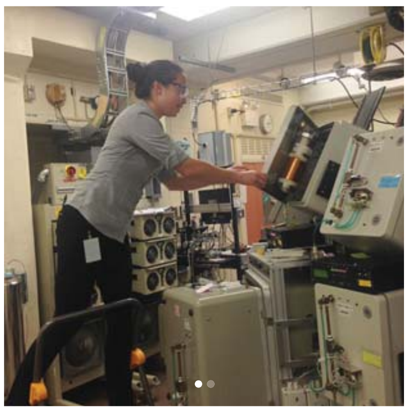
usnistgov • Following

usnistgov Just arrived at the Engineering Mechanics building. The first room that visitors encounter is the AGV lab (we also refer to it as the "low bay"). In my previous summers working at NIST, I spent most of my time in this room implementing inter-system communications for multiple robots as well as augmented reality marker-based tracking. The cameras placed across the top of the room are part of a motion capture system (also called the OptiTrack System). This is essentially the same system used to

55 likes

8 HOURS AGO

Add a comment...

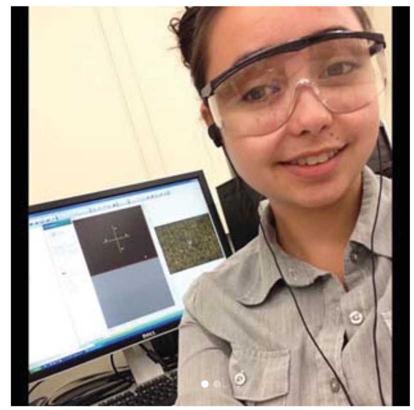


usnistgov • Following

usnistgov Hi! I'm Katrina Carlin, a rising senior at New College of Florida, and I'm doing a NISTagram Takeover today! I'm a chemistry major, and I plan to get a Ph.D. in chemistry, with an analytical and environmental focus. I'm super interested in all things "nano"--from the development of measurement science for nanoparticles in polymer composites relevant to products to the impact of nanoparticles on the service life of products, human health, and the environment.

83 likes

JULY 2



usnistgov • Following

usnistgov One of the characterization methods I use is Raman spectroscopy. This is cool because in addition to being able to see chemical changes at the surface you can also get a close up view of the nanoparticles in the polymer composite! Here's me and the sample I'm working on right now.
#takeover
#summerresearch
#nistagramtakeover
#college

69 likes

JULY 2

usnistgov • Following

usnistgov After checking my office for messages and meetings it is time to go to the high bay. I usually get to work pretty early, so my lab mates haven't arrived quite yet. In this large, industrial environment, I have a work area set up for running the robots.

This summer, I am working on extending a test method to the transporter robot shown here. This robot features a detachable cart that can hold static or

21 likes

3 HOURS AGO

SURF 2018

Students

(Alphabetical order by Last Name)

LastName	FirstName	NIST Mentor	University	OU
Aboul-Enein	Omar	Roger Bostelman	Salisbury University	EL
Abraham	Sophia	Lawrence Bassham	University of South Florida	ITL
Alberts	Gabriel	Meghan Shilling	University of Florida	PML
Anderson	Eric	Ryan Nieuwendaal	Northwestern University	MML/NCNR
Antia	Rushad	Richard Candell	University of Maryland College Park	EL
Armstrong	Paul	Wesley Griffin	University of Maryland College Park	ITL
Arnold	James	Thomas Roth	Arizona State University	EL
Arp	Gabriela	Maritoni Litorja	University of Maryland College Park	PML
Balto	Krista	John Riley	University of Delaware	MML/NCNR
Behnert	Katie	Marcus Schwaderer	PennState University	MML/NCNR
Benz	Luke	Antonio Possolo	Yale University	ITL
Bergeson	Jennifer	Behrang Hamadani	Purdue University	EL
Bernier	Shannon	Cary Presser	McDaniel College	MML/NCNR
Bhatnagar	Keshav	Marcus Mendenhall	University of Maryland College Park	MML/NCNR
Bichnevicius	Michael	Harrison Skye	PennState University	EL
Biggins	James	Sanford Ressler	University of Maryland College Park	ITL
Blick	Emily		University of Maryland College Park	CNST
Blitz	Jack	Megan Cleveland	Tulane University	MML/NCNR
Boby	Kevin	Peter Bajcsy	University of Maryland College Park	ITL
Bones	Lela	Thurston Sexton	Salisbury University	EL
Borgsmiller	Leah	Dean DeLongchamp	Northwestern University	MML/NCNR
Borres	Jeffrey	Gordon Shaw	SUAGM-Universidad del Turabo	PML
Brake	Alexis	Aaron Forster	University of Florida	MML/NCNR
Brannon	William	Lakesha Perry	Auburn University	EL
Brassel	Alexander		University of Maryland College Park	EL
Brignac	Kayla	Jennifer Lynch	University of Hawaii	MML/NCNR
Broerman	James	Arun Moorthy	University of Colorado Boulder	MML/NCNR
Burni	Faraz	Velencia Witherspoon	University of Maryland College Park	MML/NCNR
Burns	Christian	Timothy Zimmerman	Sheperd University	EL
Burrall	Hannah	Wangchun Chen	Hamilton College	MML/NCNR
Calvo	Angelo	Guodong Shao	Tennessee Technological University	EL
Cano	Alexa	Grethe Jensen	Texas A&M University Kingsville	MML/NCNR
Cao	Tiffany	Jeffrey Kim	University of Maryland College Park	MML/NCNR
Capraro	Marco	Brian Weiss	University of Maryland College Park	EL
Carangelo	Christopher	Scott Jones	Loyola University Maryland	EL
Carlin	Katrina	David Goodwin	New College Florida	EL
Cavazos	Omar	Dagistan Sahin	Texas A&M University Kingsville	MML/NCNR
Chavali	Sai Meghasena	Shannon Hoogerheide	University of Maryland College Park	PML
Chiong	Golda Meir	Derek Juba	Towson University	ITL
Clifford	Zachary	Danielle Gorka	University of Maryland Baltimore County	MML/NCNR
Collins	Ann	Jennifer Helgeson	Stevens Institute of Technology	EL
Corrigan	Alexsandra	Clare Allocca	Virginia Polytechnic Institute	SCO/TPO
Croley	Rhett	Hans Pieter Mumm	University of Kentucky	PML
Damazo	Isabel	Darwin Reyes-Hernandez	University of Pittsburgh	PML
de Oliveira	Samuel	Andrew Fairbrother	University of Central Florida	EL
Dean	Pablo	Paul Stutzman	University of Maryland College Park	EL

LastName	FirstName	NIST Mentor	University	OU
Dee	Alana	Dean Jarrett,	University of Pittsburgh	PML
Devers	Rachel	June Lau	University of Maryland College Park	MML/NCNR
Devorkin	Joshua	Susana Marujo Teixeira	University of Illinois	MML/NCNR
Dharmadhikari	Kunal	Christina Bergonzo	University of Maryland College Park	MML/NCNR
Doris	Michael	Ian Spielman	California State University Chico	PML
Eckardt	Benjamin	Ian Spielman	Bates College	PML
Eusman	Nickolas	CheeYee Tang	Worcester Polytechnic Institute	EL
Fan	Steven	Richard Rouil	University of Maryland College Park	CTL
Fastow	Eli	Cindi Dennis	University of Maryland College Park	MML/NCNR
Filteau	Jeremy	Wyatt Vreeland	Worcester Polytechnic Institute	MML/NCNR
Finlay	Ethan	Jirun Sun	Appalachian State University	MML/NCNR
Fiola	Gregory	Rodney Bryant	University of Maryland College Park	EL
Fisher	Ryan	Guodong Shao	Virginia Polytechnic Institute	EL
Fu	Matthew	Joe Kopanski	Cornell University	PML
Furrh	Jacob	Erica Kuligowski	University of Houston	EL
Galfond	Brian	Greg Vogl	Catholic University of America	EL
Garner	Jonathan	Helen Qiao	University of Maryland College Park	EL
Gezahegn	Hiwot	Wesley Garey	University of District of Columbia	CTL
Gonzalez	Shakira	Erica Stein	University of Puerto Rico	MML/NCNR
Guzman Cruz	Yinaris	Paul Zielinski	University of Puerto Rico	SCO/TPO
Hailu	Surafel	Lotfi Benmohamed	University of District of Columbia	ITL
Halam	Samantha	Davina Pruitt-Mentle	Fayetteville State University	ITL
Hall	Steven	Harold Hatch	Clemson University	MML/NCNR
Hamati	Michael	Winnie Wong	Columbia University	MML/NCNR
Higgins	Brianna	Jeremiah Woodcock	Hood College	MML/NCNR
Ho	Kevin	Gerald Fitzpatrick	University of Maryland College Park	PML
Horenberg	Allison	Carl Simon	University of Virginia	MML/NCNR
Hubbard	Joshua	Jae Hyun Kim	University of Maryland College Park	EL
Ionescu	Candice	Jennifer Marshall	Dickinson College	SCO/TPO
Isaac	Samantha	Leland Harriger	West Virginia University	MML/NCNR
Isele	Erik	Nikolai Zhitenev	University of Michigan	PML
Janzen	Eli	Ursula Kattner	Kansas State University	MML/NCNR
Jessup	Devin	Mark Stiles	George Washington University	CNST
Jiao	Sally	Harold Hatch	Princeton University	MML/NCNR
Jin	Shannon	Jacob Majikes	Columbia University	CNST
Jones	William	Gili Kaufman	University of Georgia	MML/NCNR
Kaneshige	Nathaniel	Heather Chen-Mayer	University of Hawaii	MML/NCNR
Kant	Kamryn	Nathan Mahynski	Clemson University	MML/NCNR
Keim	Klara	Styliani Alimperti	Texas Tech University	MML/NCNR
Kim	Timothy	Cuong Nguyen	University of Maryland College Park	EL
Kirsch	Dyland	Angela Hight-Walker	University of Maryland College Park	PML
Klyuev	Arsen	D. Richard Kuhn	Johns Hopkins University	ITL
Koehl	Julianna	Joel Sarapas	Lebanon Valley College	MML/NCNR
Kraus	Harrison	Marc Levitan	University of Maryland College Park	EL
Kreitman	Meir	Jordan Weaver	University of Maryland College Park	EL
Kriz	Alison	Vladimir Olesheko	University of Maryland College Park	MML/NCNR

LastName	FirstName	NIST Mentor	University	OU
Kupferschmid	Matthew	Yee-Yin Choong	Washington University St Louis	ITL
Lai	Trinny	Stephanie Watson	Regis University	EL
Lewis	Alexander	Boonserm Kulvatunyou	Trine University	EL
Li	Hengming	Lei Chen	Appalachian State University	CNST
Li	Simin	Jeremy Marvel	University of Maryland College Park	EL
Li	Qing Hai	Yan Lu	Wellesley College	ITL
Li	Xiang	Anthony Kearsley	George Mason University	ITL
Littrell	Christopher	Xiaohong Gu	Carnegie Mellon University	EL
Lopez Moralez	Alejandra	Erica Kuligowski	SUAGM-Universidad del Turabo	EL
Luu	Vanda	Li Piin Sung	University of Maryland Baltimore County	EL
Malanoski	Aidan	Ram Sriram	Reed College	ITL
Malin	Merrik	Joshua C. Bienfang	West Virginia Wesleyan College	PML
Manasiya	Siminben	Jack Douglas	University of Houston	PML
Marsh	Thomas	Mark Stiles	Hamilton College	CNST
Martin	Sabrina	Greg Gillen	University of Maryland College Park	MML/NCNR
May-Pohlman	Laurelia	Gillian Nave	University of Maryland College Park	PML
McCright	Kevin	ShengYen Li	University of Maryland College Park	MML/NCNR
McIntyre	Timothy	Marc Levitan	University of Maryland College Park	EL
McLaurin	James	Kate Klein	University of District of Columbia	PML
Meek	Stephen	Greg Cooksey	Montgomery College	PML
Miller	David	Michael Mascagni	University of Maryland College Park	ITL
Miller	Hallie	Donald Windover	Messiah College	MML/NCNR
Miranda	Angel	Erica Kuligowski	SUAGM-Universidad del Turabo	EL
Mnev	Peter	Craig Schlenoff	University of Maryland College Park	EL
Mullins	David	Daniel Hussey	University of Kentucky	PML
Murthy	Vaishnavi	Corey Stambaugh	University of Maryland College Park	PML
Musteata	Elena	David Ross	SUNY Poltechnic University	MML/NCNR
Nachega	Nicholas	Scott Rose	University of Maryland College Park	ITL
Neves	Paul	Nick Butch	University of Maryland College Park	MML/NCNR
Ng	Daniel	Mark Stoudt	Northwestern University	MML/NCNR
Nitschelm	Charlie	Steven Mates	University of New Hampshire	MML/NCNR
Nolan	John	Spencer Breiner	University of Maryland College Park	ITL
Norwood	Frederick	Nick Dagalakis	University of Colorado Boulder	EL
Okusolubo	Temiloluwa	Michihiro Nagao	University of Maryland Baltimore County	MML/NCNR
Orban	Peter	Denis Bergeron	St. Mary's College MD	PML
Orenstein	Rachel	Zachary Trautt	Northwestern University	MML/NCNR
Ott	Patrick	Qi An	University of Maryland College Park	MML/NCNR
Pandey	Abhinav	Eugene Song	University of Maryland College Park	EL
Peake	Elijah	Michelle Steves	Middlebury College	ITL
Perez	Felix	Anthony Kearsley	Texas Tech University	ITL
Pugh	Sydney	Frederick Byers	Loyola University Maryland	ITL
Resto Garcia	Angel	Paul Zielinski	SUAGM-Universidad del Turabo	SCO/TPO
Rhodd-Lee	Holland	Mandy Esch	Wellesley College	CNST
Riedel	Zachary	Katie	Clemson University	MML/NCNR
Riet	James	Shinchiro Muramoto	Virginia Polytechnic Institute and State Ur	MML/NCNR
Roa	Michael	Moneer Helu	University of Maryland College Park	ITL

LastName	FirstName	NIST Mentor	University	OU
Rodriguez Carden	Viviana	Sara Orski	Montgomery College	MML/NCNR
Roe	Emily	Lee Richter	North Carolina State University	MML/NCNR
Rogers	Emma	Mandy Esch	Tulane University	CNST
Saar	William	Erik Johnson	University of Maryland College Park	EL
Sarwat	Sumaiyah	Richard Steiner	University of Maryland College Park	PML
Schmale	Henry	Heman Gharibnejad	Millersville University Pennsylvania	PML
Seamone	Andrew	Jonathan Weigand	University of Colorado Boulder	EL
Segarra	Esteban	Shelly Bagchi	Florida Polytechnic University	EL
Serrano Torres	Luis	Randall McDermott	SUAGM-Universidad del Turabo	EL
Shah	Sejal	Ran Tao	University of Delaware	MML/NCNR
Shankar	Naveen	Kerry McKay	Carnegie Mellon University	ITL
Siegel	Jacob	Stephen Eckel	University of Maryland College Park	PML
Smith	Ryan	Jason Hattrick-Simpers	University of Houston	MML/NCNR
Sorra	Justin	Natascha Milesi-Ferretti	University of Maryland College Park	EL
Sredenschek	Alexander	Christina A. Hacker	Messiah College	PML
Stakhovsky	Kirill	Dagistan Sahin	University of Maryland College Park	MML/NCNR
Stauffer	Eileen	Zeeshan Ahmed	University of Maryland College Park	PML
Stemple	Carrie	Amy Xu	Wilson College	MML/NCNR
Steves	Paul	Kevin Mangold	Washington College	ITL
Strogen	Nicholas	Michael Riley	West Virginia University	MML/NCNR
Sturek	Claire	Diane Bienek	Catholic University of America	MML/NCNR
Suczewski	Gregory	Paul Kienzle	Middlebury College	MML/NCNR
Sun	Xinran	Yan Lu	University of Michigan	EL
Swamykumar	Prateek	Daniel Siderius	University of Maryland College Park	MML/NCNR
Tamayo Claro	Cesar	William Bernstein	Arizona State University	EL
Taylor	Zachary	Paul Zielinski	North Carolina State University	SCO/TPO
Todd	Alexander	Daniel Hussey	Indiana University	PML
Tovcimark Jr	Stephen	Liya Yu	SUNY Poltechnic University	CNST
Tran	Ha	David Bunk	University of Maryland College Park	MML/NCNR
Trowbridge	Julia	Babak Nikoobakht	Colorado State University	MML/NCNR
Turner	MaKayla	Eric Cockayne	Boise State University	MML/NCNR
Underwood	Ryan	Thomas Gnaupel-Herold	University of Central Florida	MML/NCNR
Vega Nogales	Alejandro	Timothy Blattner	University of Puerto Rico	ITL
Vejalla	Varsha	Andrew Rukhin	University of Virginia	ITL
Vincent	Galen	Nils Persson	Colorado School of Mines	MML/NCNR
Wages	Hunter	Solomon Woods	Wofford College	PML
Walsh	John	Vance Payne	University of Maryland College Park	EL
Walz	Francis	Joseph Tan	Towson University	PML
Warner	Morgan	David Griffith	Tennessee Technological University	CTL
Waysack	Joseph	Judith Terrill	Millersville University Pennsylvania	ITL
Weiss	Abdullah	Dagistan Sahin	Texas A&M University Kingsville	MML/NCNR
Wernsing	Galahad	Jared Wahlstrand	Worcester Polytechnic Institute	PML
Weyhmiller	Aubrie	Tim Barvitskie	Rowan University	MML/NCNR
Whiting	Zachary	Ron Tosh	West Virginia Wesleyan College	PML
Wigham	Caleb	Ryan Murphy	Texas Tech University	MML/NCNR
Williams	Richard	Kerry McKay	University of Maryland College Park	ITL

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Wilson	Abigail	William Ratcliff	Tufts University	MML/NCNR
Winetrout	Jordan	Alexander Borque	University of Southern Mississippi	MML/NCNR
Wu	Sulan	Hua-Jun He	Oberlin College	MML/NCNR
Xiong	Xinyu	Vincent Hu	City College of New York	ITL
Yagodich	Julie	Daniel Siderius	Frederick Community College	MML/NCNR
Yoon	David	Paul Salipante	Northwestern University	MML/NCNR
Young	Candace	Christina Jones	Chicago State University	MML/NCNR
Zambrotta	Ryan	Fred Phelan	Northwestern University	MML/NCNR
Zhu	Jesse	John Lu	Cornell University	ITL
Zong	Kevin	Oliver Slattery	University of Maryland College Park	ITL
Feeney	Patrick	Kevin McGrattan	University of Rhode Island	


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