
NIST SURF 2019

Greetings!

On behalf of the Director's Office, it is my pleasure to welcome you to 2019 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 160 participants from 100 universities engaging in research projects in all the 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, #2019SURFColloquium.

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 K. 2

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
Communications Technology Lab	David Griffith
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	Derek Juba
Information Technology Lab	Yolanda Bursie
Material Measurement Lab	Andre Striegel
Material Measurement Lab	Amanda Forster
Material Measurement Lab	Jessica Staymates
NIST Center for Neutron Research	Julie Borchers
NIST Center for Neutron Research	Joseph Dura
Physical Measurement Lab	Joseph Kopanski
Physical Measurement Lab	Richard Steiner
Physical Measurement Lab	Uwe Arp
Physical Measurement Lab	Maritoni Litorja
Technology Partnership Office	Paul Zielinski
Standards Coordination Office	Nathalie Rioux

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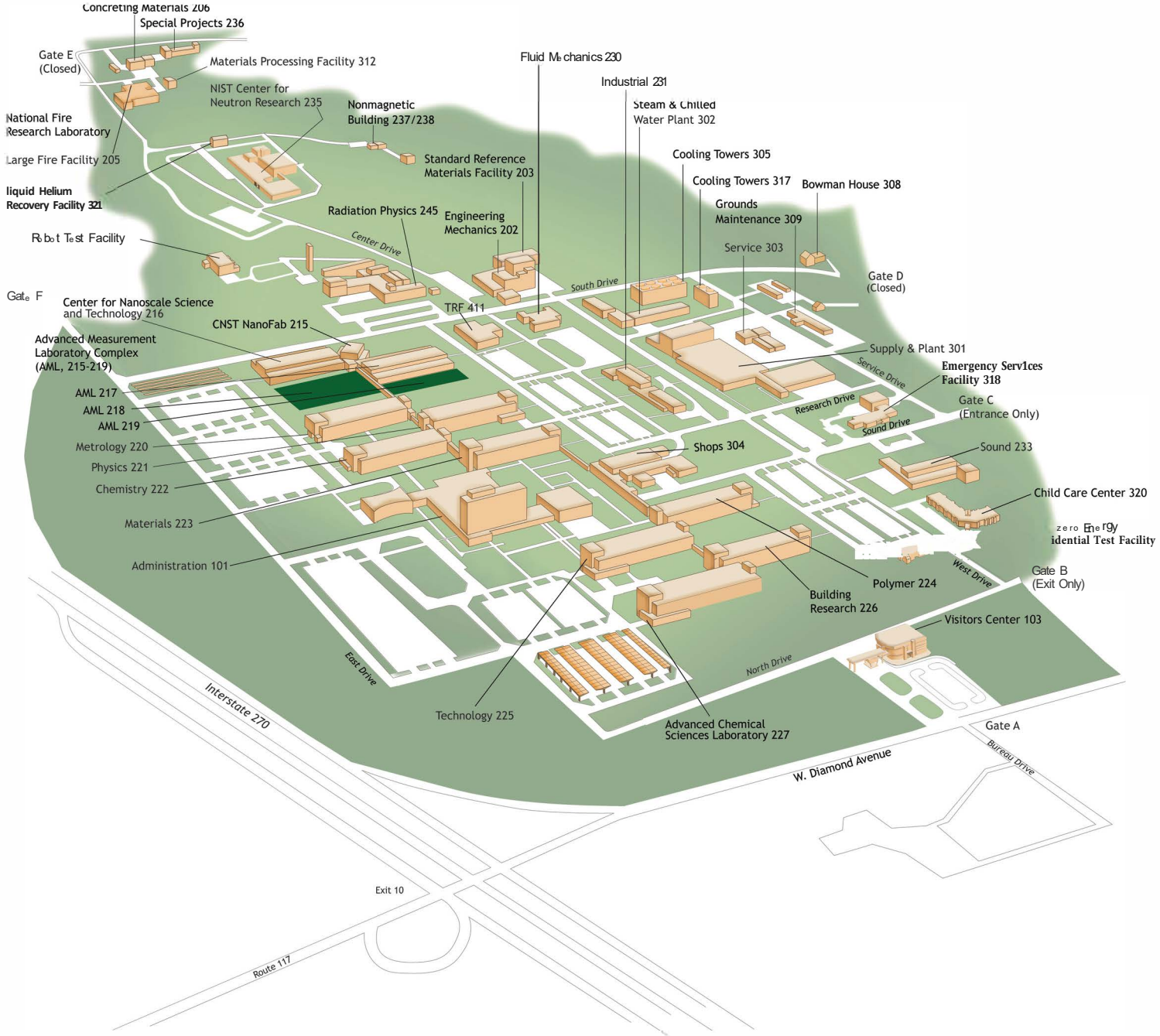
Table of Contents

Campus Map


Concreting Materials 206
Special Projects 236
Gate E
(Closed)
Materials Processing Facility 312
NIST Center for
Neutron Research 235
Nonmagnetic
Building 237/238
National Fire
Research Laboratory
Large Fire Facility 205
liquid Helium
Recovery Facility 321
Standard Reference
Materials Facility 203
Radiation Physics 245
Engineering
Mechanics 202
Robot Test Facility
Center Drive
Fluid Mechanics 230
Industrial 231
Steam & Chilled
Water Plant 302
Cooling Towers 305
Cooling Towers 317
Bowman House 308
Grounds
Maintenance 309
Service 303
South Drive
Gate D
(Closed)
Gate F
Center for Nanoscale Science
and Technology 216
TRF 411
CNST NanoFab 215
Advanced Measurement
Laboratory Complex
(AML, 215-219)
Supply & Plant 301
Service Drive
Emergency Services
Facility 318
AML 217
AML 218
AML 219
Research Drive
Gate C
(Entrance Only)
Sound Drive
Metrology 220
Physics 221
Chemistry 222
Shops 304
Sound 233
Child Care Center 320
Materials 223
Zero Energy
Residential Test Facility
Administration 101
West Drive
Gate B
(Exit Only)
Polymer 224
Building
Research 226
Visitors Center 103
East Drive
North Drive
Interstate 270
Technology 225
Advanced Chemical
Sciences Laboratory 227
Gate A
Bureau Drive
W. Diamond Avenue
Exit 10
Route 117

August 5, 2019
SURF Colloquium Plenary Session
Location: Green Auditorium in the Administration Building 101

Time	Agenda
9:30A	**Welcome** Speaker**:** Dr. Walter Copan Under Secretary of Commerce for Standards and Technology NIST Director
9:40A	**Moderator**: Dr. Brandi Toliver Managing SURF Program Director
9:45A	**CTL** Presenter: Emma Bradford Title of Talk: Simulation of a GAA-GAA Coexistence Scheme in the CBRS Band
10:05A	**EL** Presenter: Jared Kaplan Title of Talk: Health Degradation Assessment for Robotic Manufacturing
10:25A	**ITL** Presenter*:* Elisabeth Landgren Title of Talk: Quantum Dots and Virtual Reality: The Pursuit of Intuitive Data
10:45A	Break
11:00A	**MML** Presenter: Ethan Finlay Title of Talk*:* Approaches to Minimize Polymerization Stress in Dental Resin Composites
11:20A	**NCNR** Presenter*:* Emily Blick Title of Talk: Long-Term Vesicle Stability for Liposomal Nanomedicines
11:40A	**PML** Presenter: Amberly Ricks Title of Talk: Electrical Characterization of DNTT-based Organic Field Effect Transistors
Noon	**Lunch**

Monday, August 5, 2019 Parallel Session Schedule					
	Lecture Room A	**Lecture Room B**	**West Square**	**Heritage Room**	**Lecture Room D**
	MML/NCNR_Comput. Science	**MML/NCNR_MatSci**	**ITL**	**EL**	**PML**
Time	Moderator: Dr. William Brad O'Dell	Moderator: Prof. Mohamad Al-Sheikhly	Moderator: Tim Burns	Moderator: TBD	Moderator: TBD
1:30 PM	*Katrina Rupert:* Getting the Kinks Out: Reducing Disulfide Bonds for Protein Analysis	*Julie Colon-Martinez* : Selectivity Prediction on Binary Gas Absorption of CO2/N2 on Zeolite Reference Materials	*Roberto Rafael Gorbea Finalet* : Testing Quantum-Inspired Classical Algorithms	*Varsha Vejalla* : Business Interruption and Recovery Following a Disaster.	*Jack Fletcher* : Lithium-7 Gray Molasses
1:50 PM	*Caitlin Darling:* The role of Copper and Nickel in lipid oxidation relevant for antimicrobial action	*Jinsung Lee* : Determining Optimal 3D Configuration of Porous CO2 Reduction Catalysts	*Kevin Zong* : Network Management System Towards the Platform for Quantum Network Innovation	*Nicolas Aguilar* : Hazard Characterization & Facility Analysis in Puerto Rico After Hurricane Maria	*Franklin Nicolas Gavilanez Villalta* : Intercomparison Study of Optical Measurement Methods for Toolmark Analysis
2:10 PM	*Nathan Gill:* Understanding ClpS N-Terminal specificity through combined simulation and experiment	*Eli Fastow* : Cross-comparison and Validation of Complementary Analytical Methods to Detect Lithium	*Angelica Lin* : Applied Chemometric Methods for Monoclonal Antibody Classification	*Dianeliz Ortiz Martes* : Documenting Characteristics of Hospitals Impacted by Hurricane Maria in Puerto Rico	*Kathryn Gill* : Photonic Biochemical Sensors and their use
2:30 PM	*Joshua Price:* Calibrating Deuterium Incorporation into Green Fluorescent Protein Expressed in the Yeast Komagataella phaffii	*Ryan Smith* : Correlating Structural and Functional Properties with Amorphicity of Alloys	*Daniel De Leon* : Fractals derived from constrained optimization techniques using Newton's Method	*Sarah Morgan* : Identifying Consensus Indicators and Measures to Help Assess Community Resilience	*Peter Orban* : Improving Stack Flow Measurements by Making Them Faster and More Accurate
2:50 PM	*Allison Horenberg* : Measuring Cell Viability in Collagen Scaffolds	*Huilang Chen* : Blade-coated In2O3/ZnO bilayer heterostructures	*Lily Northcutt* : Modeling First Passage Brownian Motion using Walk on Spheres Method	*Clio Chen* : Development of Adaptable Concrete Structures Using Non-Newtonian Fluids	*Tojo Rabemananjara* : Camera and Projector Synchronization to Improve SI-MMI Speed and Efficiency
3:10 PM	Break	Break	Break	Break	Break

Monday, August 5, 2019 Parallel Session Schedule (continued)

	Lecture Room A	Lecture Room B	West Square	Heritage Room	Lecture Room D
	MML/NCNR_Comput. Science	**MML/NCNR_MatSci**	**ITL**	**EL**	**PML**
	Moderator: Dr. Monique Johnson	Moderator: Dr. Brandi Toliver	Moderator: TBD	Moderator: TBD	Moderator: TBD
3:20 PM	*Darnell Harris* : Design and Production of Viral Scaffolds for Cryo-EM	*Rajashow Parajuli* : Predicting Protein Properties with Machine Learning	*Justin Slud* : Towards Integrating Virtual Reality with NIST's Digital Library of Math Functions	*Quichawna Bryant* : Synthesis and Characterization of Cement Mineral Phases	*Hristiana Stoynova* : Reducing Uncertainties in Carbon Storage and Fluxes: A Focus on Japanese Stiltgrass
3:40 PM	*Oriana Ovide* : Assessment of Elemental Homogeneity in Modern Glass micro-XRF for forensics	*Simin Manasiya* : Using Atomistic Simulations to Relate Local Molecular Dynamics and Fluorescence Lifetime in a Damage Sensing Dye	*Peter Stein* : CHIMeS: Developing a Common CAVE and Web-Based Virtual Reality Menu System	*Riley MacLaren* : Corrosive Degradation in Concrete Infrastructure with Low-Carbon Steel and Nitinol	*Hunter Wages* : Thermal Imaging: An End-to-End Simulation
4:00 PM	*Winnie Tran* : Combining LC-MS and ELISA for Quantification of Allergenic Milk Protein in Food	*Jacob Hechter* : Interatomic Potentials for Calculating Diffusion Behavior	*Linus Ge* : On generating functions for q-inverse polynomials in the q-Askey scheme	*Clare Chan* : Rheological characterization of 3-D printable cement paste	*Arjun Agarwal* : Vacuum Ultraviolet Fourier Transform Spectroscopy of Iron Group Elements
4:20 PM	*Ava Farahbakhsh Darabi* : Developing Oral Sensors Based on Glucose and pH Levels	*Eleanor Kelman* : Finding High Condutive Transparent Oxides with Active Learning	*Eve Fleisig* : A GUI for Evaluation of Distance Metrics on Heterogeneous Data Sets	*Lindsay Hutton* : Polymer Modified Cements for 3-D Printing Applications	*Caroline Azadze* : Performance Measurements of Smart Sensor in Smart Grid
4:40 PM	*Joelle Marchiani* : Chemical Weathering and Additives in Plastic Marine Debris in the Hawaiian Islands (pre-recorded)			*Mariana Bueno* : Influence of particle size ratio on suspension rheology with a bimodal size distribution	*Julia Codere* : Analysis of the Harmonics of Distorted Power Waves from Smart Watt-hour Meters
5:00 PM					

Tuesday, August 6, 2019 Parallel Session Schedule					
	Lecture Room A	**Lecture Room B**	**Lecture Room C**	**Heritage Room**	**Lecture Room D**
	MML/NCNR_Comput. Science	**MML/NCNR_MatSci**	**ITL**	**EL**	**PML**
Time	Moderator: TBD	Moderator: Dr. Guebre Tessema , NSF	Moderator: Derek Juba	Moderator: TBD	Moderator: Zachary Levine
9:00 AM	*Jonah Tash:* Dynamic Taxonomies for Root & Rule Based Language Trees	*Mark Zic:* Neutron Scattering Study of a Triplet Superconductor	*Gerson Kroiz* : Exploiting Coarse-Grained Parallelism in Numerical Linear Algebra Routines	*Laura Mundy* : Establishing a New Standard Reference Portland Cement Clinker for Phase Analysis using Scanning Electron Microscopy	*Robert Kauffman* : Automated Fiber Coupling with Machine Learning Optimization
9:20 AM	*Noah Smith:* Enabling FAIR Data Principles for High-Throughput Experimental Data	*Spencer Rodgers* : Probing Anomalous Field-Expulsion in Superconductor/ Ferromagnetic Thin Films	*Henok Tasissa* : Hedgehog Generator: Tool used to generate boilerplate code	*Anisa Moore* : Hydration Reactions in Micro-structures	*Caitlin Lee* : Improvements to the Dual Source Bridge System for Calibration of High Resistance Standards
9:40 AM	*Thomas Bina* : Development of the Microscopy Laboratory Information Management System	*Lizabeth Quigley* : Depth Dependence of Skyrmions in Thin Films	*Kevin Boby* : Deep Learning: Is more training data always better?	*Mariam Hasan* : Degradation of Fiber-Reinforced Polymer (FRP) Composites Used as Building Retrofits	*Guadalupe Quirarte* : Developing and optimizing the optical system for observing transitions between metastable states of highly charged ions created inside a mini-EBIT
10:00 AM	*Yuke Wang* : Feature Engineering for Small Angle Neutron Scattering A.I.	*Malgorzata Psurek* : Breaking up the crystal lattice to improve superionic conductivity	*Cameron Smith* : Creating a software client to show conformance of healthcare info - HL7 v2 Standard	*Zachary Werrmann* : Analysis of the Polymeric Degradation of Solar Module Backsheets	*Macrae Smith* : Providing a Digital Framework for Testbed Research With LabVIEW
10:20 AM	*Samuel Phillibe:* Developing a Virtual Instrument for a High-Throughput Thermal Analysis Instrument	*Candyce Collins* : When Polymers Meet: Self-Assembled Amphiphilic Diblock Copolymers		*Nina Lau* : Accelerated Weathering of Polyester Using Integrating Sphere Technology	*Eli Weissler* : Photon Echo Based Quantum Memory
10:40 AM	Break	Break	Break	Break	Break

Tuesday, August 6, 2019 Parallel Session Schedule (continued)			
	Lecture Room A	**Lecture Room B**	**Heritage Room**
	MML/NCNR_ChemBio	**MML/NCNR_MatSci**	**EL**
Time	Moderator: Dr. Anthony Kotula	Moderator: TBD	Moderator: TBD
11:00 AM	*Klara Keim* : Elucidating the Effect of Extracellular Matrix Stiffness in Oral Microvasculature Utilizing Microfluidic Devices	*Julianna Price* : Oral Insulin Delivery via Microencapsulation	*Samuel Riddle* : Quantitative Visualization of Crack Formation in Polymer Backsheet Materials
11:20 AM	*Fjorela Xhyliu* : NAC rescues dental pulp cells exposed to toxic dental monomer	*Washat Roxanne Ware* : Using Viscoelastic Properties of Polymer and Lipid to Study the Cell Membrane	*Alexander Conrad* : Investigating PVC Reciprocity Throughout SPHERE Irradiance
11:40 AM	*Nidhi Vantair:* Developing a Candidate Reference Material to Assess DNA Extraction Efficiency	Racheal Spruill: SURFing with Green Tea: What Neutrons Read in Tea Leaves	*June Greenstein* : Tracking Cable Degradation in Nuclear Powerplants
12:00 PM	*Usmaan Siddiqui* : Self Assembly and Solution Structure of Supramolecular Bottlebrush Polymers	*Marshall Nakatani* : Capillary µRheoSANS: Lipid Vesicle Nanostructure and Rheology at High Shear	*Donald Truong:* The Unknown Factors of Heating and Cooling Air
12:20 PM		*Emma Rogers* : The Development of Bilayer Overtone Analysis for Measuring Protein and Ion Activity	*Sriniket Rachuri* : Using HVAC-Cx in the Building Commissioning Process
12:40 PM	Lunch	Lunch	Lunch

Tuesday, August 6, 2019 Parallel Session Schedule (continued)			
	Lecture Room A	**Lecture Room B**	**Heritage Room**
	MML/NCNR_MatSci	**MML/NCNR_MatSci**	**EL**
Time	Moderator: Dr. Carrie Campbell	Moderator: TBD	Moderator: TBD
1:30 PM	*Adam Robinson* : Neural Network interatomic potentials: Feature selection and property sensitivity	*Andrew Seamone* : Thermal-Hydraulics Feasibility for an Optimized Ultra-Compact Nuclear Reactor	*Tejas Dinesh* :Optimizing Heat Exchangers
1:50 PM	*Nina Agrawal* : Characterizing the Cooperative Motion in Condensed Fluids Using Machine Learning	*Hamna Chaudhry* : NBSR Reactor Plant State Predictor	*Zynyl Castor* : Incorporation of BlenderGIS into FDS modeling workflow
2:10 PM	*Julie Yagodich* : Data Acquisition and Image Analysis of Small Angle Light Scattering	*Disha Das* : Performing Human Factors Analysis on Nuclear Reactor Console with Mixed Reality	*Devon Suarez* : Optimization for High Performance Computing
2:30 PM	*Julia Danischewski:* Finding the Binding: Synthesis and Dynamic Light Scattering Analysis of Polyelectrolytes	*Joseph P Rath III* : The Applications of Artificial Intelligence in Neutron Diffraction Analysis	*Genevieve Tan* : Assessing the Smoldering Propensity of Wood Exposed to Direct Contact Heating
2:50 PM	*Nick D'Antona* : Analysis of electrochemically doped polymer thin films via in situ ellipsometry	*Gamitha Wijekoon* : Neutron Tomography and Simulation of Compton Imaging	*William Saar* : Pursuing Improved Solid Pyrolysis Models
3:10 PM	*Lu Song* : Evaluating mechanical and chemical properties of polydimethylsiloxane using rheo-Raman microscope		*Sebastian Arana* : Modeling Wildland Urban Interface Fires on a Standard Parcel
3:00 PM	*Chad Hite* : Elucidating the Role of Hinge Mechanics on Impact Mitigation		*Adam Lenker* : Web-Based Data Augmentation of 360-Degree Video for Fire Research
3:20 PM	Break	Break	Break

Tuesday, August 6, 2019 Parallel Session Schedule (continued)				
	Lecture Room A	**Lecture Room B**	**Heritage Room**	**Lecture Room C**
	PML	**ITL**	**EL**	**TPO**
Time	Moderator:Dr. Joseph J. Kopanski	Moderator: Dr. Michaela Iorga	Moderator: TBD	Moderator: TBA
3:30 PM	*Adam Brewer* : Programming Automated Programming	*Thomas Hayes* : Measuring Public Awareness of Cybersecurity Careers	*Steven Mallia* : A case study for modeling machine tool systems using standard representations	*Samantha Gibson* : Technology transfer development at NIST and the Technology Discovery Office
3:50 PM	*Mark Yves Gaunin* : Atomic-Scale Quantum Plasmonics	*Glen Joy* : Securing the Energy Sector through Standards-Based Cybersecurity Architectures	*Ian Macke* y: HDF5 and DREAM.3D Applications for Additive Manufacturing	*Sue Lee:* Technology transfer development at NIST and the Technology Discovery Office
4:10 PM	*Liza Gunther* : Atom-Based Silicon Quantum Electronics	*Jesse Zhu* : User interface development for Root and rule (R&R) based system for curating, indexing and searching documents	*Daniel Hartenstine* : Creating A Data Processing Pipeline Architecture For Manufacturing Systems	
4:30 PM	*Matthew Ishimaru* : Stable Foundations for Quantum Computing: Characterizing van der Waals Materials	*Shayer Parvez* : Revamping Health Care Through Rule-Based Expert AI Systems	*Christina You* : Using Neural Networks to Detect Kitchen Cooktop Pre-Ignition	
4:50 PM	*Jesus Perez* : COMSOL Simulations of Electromagnetic Test Structures	*Matthew Kupferschmid* : Data Analysis of Cooktop Sensors	*Isaac Rose* : High-precision Stereo Camera Calibration and Assessment	
5:10 PM				

Wednesday, August 7, 2019 Parallel Session Schedule			
	West Square	**Lecture Room B**	**Lecture Room C**
	EL	**ITL**	**PML**
Time	Moderator:TBA	Moderator: Derek Juba	Moderator: Daniel S. Hussey
9:00A	*Adam Wathieu* : Investigating the Standardization of Work Volume for Robotic Manipulators	*Sydney Pugh* : Developing Effective Test Strategies for Cryptographic Algorithm Implementations	*Amber Meyers* : Ultrafast laser spectroscopy to study photodynamics of asymmetric hydrogenases
9:20A	*Kyle Shreve*: Squareness Testing of Machine Tool Linear Axes Based on Inertial Measurements	*Temur Saidkhodjaev* : Verified Timestamping	*Russell Schwartz* : Closed loop update algorithm for Neuromorphic AI Accelerators
9:40A	*Esteban Segarra Martinez* : Adaptive Metrics and Performance Analysis Tool for Human-Robot Interaction	*Damien Beecroft* : Stream Learning for Min-Entropy Prediction	*Benjamin Wade* : High Bit Rate Solid State Quantum Random Number Generation
10:00A	*Steven Fang* : Industrial network interface for railroad operation simulation framework	*Richard Williams Jr* : The Effect of Different Bias Estimation Methods on Linear Cryptanalysis	*Michael Doris* : Eliminating Thermal Gradients For Neutron Interferometry
10:20A	*Thomas Wrona* : Simulation and Data Analysis for Cybersecurity on Industrial Control Systems	*Caleb Robertson* : Analysis of the Current Security Infastructure Partaining to Small Unmanned Aerial Systems	*Thomas Marsh* : Analyzing spot weld strain using Neutron Bragg Edge Tomography
10:40A	Break	Break	Break

Wednesday, August 7, 2019 Parallel Session Schedule (continued)			
	West Square	**Lecture Room B**	**Lecture Room C**
	EL	**ITL**	**PML**
Time	Moderator:TBA	Moderator: Lotfi Benmohamed	Moderator: TBA
11:00 AM	*David Umansky* : Analysis of Surface Finish in Laser Powder Bed Fusion Additive Manufacturing	*Mason Rhodes* : Dynamic Cache Management with Network-Wide Capacity Constraint	*Gillian Lee* : Using Potentiometry to Determine the Purity of Standards for Electron Paramagnetic Resonance (EPR) Spectroscopy
11:20 AM		*Daniel Tokarz* : Dveloping a Graph Database to Evaluate/Analyze Cyber Incidents	*Elieser Mejia* : Nanoscale Engineering of Optical Resonances using Metasurfaces
11:40 AM		*Kevin Zong* : NVD, CPEs, and CVEs: Maintaining a Searchable Vulnerability Database	*Michelle Morris* : Field Effect Transistors Offer a New Level of Sensitivity for Biological Measurements
12:00N		*Eric Liu* : Hardware-Based Security Measures for Virtual Machines	*Nikita Podobedov* : Repeated Flow Cytometry Measurements Along a Single Microfluidic Channel in an Optofluidic Chip
12:20P		*Joseph Converse* : The Implementation of Side-of-Fringe Locking Techniques to Reduce the Frequency Drift of a CW Laser	*Heriniaina Rakotomanana* : Fabrication of a Helium Ion Machined Nanochannel Device
12:40P			*Holland Rhodd-Lee* : Measuring Endothelial Molecular Transport Using a Pumpless Microfluidic System

CTL


WELCOME
TO
SURF
NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

SURF

CTL SURF Participants

First Name	Last Name
Emma	Bradford
Yu Xuan	Huang

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Emma Bradford		
Academic Institution: University of Cincinnati	**Major:** Computer Science & Anthropology	
Academic Standing (Sept. '19):	3rd year of 5 year program	
Future Plans (School/Career):	Go to graduate school to get my PhDs and become a Professor	
NIST Laboratory, Division, and Group:	Communications Technology Laboratory, Wireless Network Devision	
NIST Research Advisor:	Dr. Anirudha Sahoo	
Title of Talk:	Simulation of a GAA-GAA Coexistence Scheme in the CBRS Band	

Abstract:

Spectrum in the Citizens Broadband Radio Service (CBRS) has been made available for commercial use by the Federal Communications Commission (FCC) to address spectrum crunch in the sub 6 GHz band. The CBRS has three tiers: the current incumbents operate in tier 1 with the highest priority; the Priority Access License users belong to tier 2 and have medium priority; and the General Authorized Access (GAA) users operate in tier 3 with the lowest priority. The FCC rules specify that the GAA users must cooperate with each other to minimize interference and increase spectral efficiency. As a result, the Wireless Innovation Forum has proposed three approaches. The focus of this project is the third approach, named Approach 3.

At the core of the approaches is the interference graph. The interference graph is a graph where the CBSDs are the nodes and the edges represent significant interference between two CBSDs. A group of CBSDs can form a Coexistence Group (CxG) that manages interference among its member CBSDs.

Approach 3 proposes an algorithm for a cluster of CBSDs that tries to maximize bandwidth allocated to CxGs. The algorithm finds the number of unique CxGs that a CBSD and its neighbors belong to. If this number is one, then the CBSD is allocated 100 % of the bandwidth. The CBSD is allocated 50 % of the bandwidth if the number is two and so on.

In this project, Approach 3 will be implemented around the already existing code that has been developed for analyzing Approach 1. The implementation will use terrain and land cover data of the USA and will be tested at San Diego and Virginia Beach. Performance of Approach 3 will be evaluated at different deployment densities using two different propagation models: the Irregular Terrain Model (ITM) and the Hybrid Model.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Yu Xuan Huang		
Academic Institution: The City College of New York	**Major:** Computer Science & Mathematics	
Academic Standing (Sept. '19):	Graduated	
Future Plans (School/Career):	Graduate School	
NIST Laboratory, Division, and Group:	Communications Technology Laboratory, Wireless Networks Division	
NIST Research Advisor:	Tanguy Ropitault	
Title of Talk:	3D Visualizer for Millimeter Wave Communication	

Abstract:

The Institute of Electrical and Electronics Engineers (IEEE) is responsible for developing and maintaining Wireless Local Area Network (WLAN) standards, also known as WiFi. One of the latest WiFi operations is the WiGig standards, allowing consumer wireless communication at multi-gigabit speeds. WiGig operates at the 60 GHz frequency band, as opposed to the 2.4 GHz and 5 GHz bands traditionally used in WiFi. The most recent upgrade to WiGig is the IEEE 802.11ay standard, which supports transmission rates up to 100 Gbit/s, thanks to the introduction of Multiple-Input and Multiple-Output (MIMO) antennas and channel bonding/aggregation. NIST is currently implementing the components of the IEEE 802.11ay protocol in ns-3, a system-level network simulator. Our project focuses on building 3D visualizer tools via a Graphical User Interface (GUI) to analyze key components of the protocols. Our key tasks were to introduce new functionalities and to optimize the performance. A 3D visualizer allows us to identify and evaluate the beam training and tracking algorithms performance by analyzing the chosen antenna patterns dynamically, depending on the 3D geometry of the environment and the multi-path components between a transmitter and a receiver.

EL

EL SURF Participants

First Name	Last Name
Nicolas	Aguilar Aigner
Sebastian	Arana Vasquez
Quichawna	Bryant
Mariana	Bueno
Zynyl Anwynn	Castor
Clare	Chan
Clio	Chen
Alexander	Conrad
Tejas	Dinesh
Steven	Fang
June	Greenstein
Daniel	Hartenstine
Mariam	Hasan
Lindsay	Hutton
Jared	Kaplan
Nina	Lau
Adam	Lenker
Ian	Mackey
Riley	MacLaren
Steven	Mallia
Anisa	Moore
Sarah	Morgan
Laura	Mundy
Dianeliz	Ortiz Martes
Sriniket	Rachuri
Samuel	Riddle
Isaac	Rose
William	Saar
Esteban	Segarra Martinez
Kyle	Shreve
Devon	Suarez
Genevieve	Tan
Melissa	Tensa
Donald	Truong
David	Umansky
Varsha	Vejalla
Adam	Wathieu
Zachary	Werrmann
Thomas	Wrona
Christina	You

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Nicolas Aguilar		
Academic Institution: Montgomery College	**Major:** General Engineering	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Obtain a master's degree & consider doing a PhD. Pursue a career in engineering.	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Material & Structural Systems Division, Structures Group	
NIST Research Advisor:	Marc Levitan	
Title of Talk:	Hazard Characterization & Facility Analysis in Puerto Rico After Hurricane Maria	

Abstract:

On September 20, 2017, the island of Puerto Rico was struck by Hurricane Maria, a category 4 hurricane that reached speeds of 249.4 km/h (155 mph) and destroyed much of the island's infrastructure. In 2018, NIST initiated a multi-year program under the National Construction Safety Team (NCST) Act aimed towards assessing how critical buildings and emergency communication systems performed during the storm. The main goal of the program is to eventually make recommendations to improve building codes, standards and practices in order to make communities across America more resilient to hurricanes and other natural disasters.

The first component of my project consists on the characterization of the multiple hazards associated with Hurricane Maria, including rainfall, storm surge, flooding, landslides, and extreme winds, using data obtained from NIST and other federal agencies. The second component is the identification and geolocation of certain critical facilities, including buildings used as hurricane shelters and telecommunication towers. The geographic information systems ArcGIS and Google Earth were used to map the hazards and extract hazard characteristics at locations for each critical facility, in order to analyze and understand facility performance and damage in the context of the hazard level experienced at each site. This data will eventually be used to assist in the selection of buildings for wind tunnel testing.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Sebastian Arana		
Academic Institution: University of Maryland College Park	**Major:** Mechanical Engineering	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	I plan to finish my undergraduate studies, after that I'm not sure.	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Wildland Urban Interface Fire Group	
NIST Research Advisor:	Rik Johnsson, Kathy Butler, Kuldeep Prasad	
Title of Talk:	Modeling Wildland Urban Interface Fires on a Standard Parcel	

Abstract:

Wildland urban interface (WUI) fires have been the cause of extensive property damage in high-risk areas such as California. Some key factors that enable these fires to spread are winds, terrain, and fuel. To ensure the safety of life and property, it is necessary to understand how structural and vegetative fuels impact fire spread from wildland ecosystems to urban communities. The Fire Dynamics Simulator (FDS) modeling software has been developed by NIST to model the behavior of fire using a computational fluid dynamics approach. FDS has been used extensively to model fire spreads, and has the potential to study WUI fires on the scale of a neighborhood or greater. PyroSim, developed by Thunderhead Engineering, is a graphical user interface for FDS that shortens the time for building complex models for FDS by allowing the user to import CAD models.

The approach for this project is to develop a fire model of a Standard Parcel. The Standard Parcel is a property lot 0.25 acres in size, containing a house, a fence, and vegetation. Other combustible objects, such as a woodpile or shed, may also be included, and additional Standard Parcel sizes of 1/2 and 1 acre may be added in the future. For the initial house design, NIST's Net-Zero Energy Residential Test Facility (NZERTF) was selected. After development of the model, the Standard Parcel will be burned in various scenarios, including different ignition locations and wind conditions. Performing these tests allows identification of the different ways in which fire can spread to a house from nearby combustible materials and objects. The results may suggest steps that can be taken to protect a property from a WUI fire.

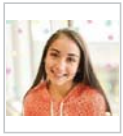
SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Quichawna Bryant		
Academic Institution:	East Carolina University	**Major:**	Mechanical Engineering
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	Graduate studies in aerospace engineering and chemical engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems, Inorganic Materials		
NIST Research Advisor:	Jeffrey Bullard		
Title of Talk:	Synthesis and Characterization of Cement Mineral Phases		

Abstract:

Portland cement, the primary component in concrete, is developed by mixing limestone and clay in specific proportions and heating the mixture at very high temperatures in a tilted, rotating kiln. This process creates what is called clinker, which is then ground with gypsum to stabilize it. The individual components of the clinker, known as phases, are termed alite, belite, aluminate, and ferrite. Determining how these phases react alone with water aids in understanding the properties of Portland cement as it sets and how each phase contributes to these properties. Alite is the most abundant in cement at roughly 45% to 70%. It is tricalcium silicate, abbreviated as C3S. This phase is very reactive early on and gives the cement much of its strength. The project focused on synthesizing alite individually and characterizing it in comparison with previously obtained samples. Thermogravimetric analysis (TGA) was done to determine the correct amounts of quartz (SiO2) and limestone (CaCO3) needed. Calcination of the limestone was necessary to evaporate carbon dioxide, leaving behind quicklime (CaO) for the actual synthesis. This process resulted in a 43.9% loss by weight of carbon dioxide (CO2) from the limestone. The quartz was determined to have a purity of 99.5%. Based on the required 3:1 stoichiometric ratio between quicklime and quartz for the synthesis, the mass ratio for synthesis was determined to be 4.974 g CaCO3 to 1 g SiO2. These components were mixed together, calcined at 1000°C for one hour, and subsequently sintered at 1600°C for two hours. The resulting product was then quenched in a steel receptacle. Another sintering was done directly at 1600°C for two hours before analyzing the C3S. X-ray diffraction (XRD) and scanning electron microscopy (SEM) were then used to characterize the purity of the phase. If not over 99%, subsequent sintering was done to achieve this conversion percentage.



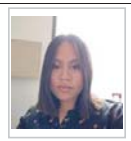
SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Mariana Bueno		
Academic Institution:	University of Maryland, Baltimore County	**Major:**	Mechanical Engineering
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	Attend graduate school		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials & Structural Systems Division, Inorganic Materials		
NIST Research Advisor:	Nicos Martys		
Title of Talk:	Influence of particle size ratio on suspension rheology with a bimodal size distribution		

Abstract:

The National Institute of Standards and Technology (NIST) develops Standard Reference Materials (SRM) that are used to calibrate instruments. There already have been two SRMs developed for the concrete industry to calibrate rheometers used to study the flow of cementitious materials. One certifying the yield stress and plastic viscosity for a cement paste and the other for a mortar. A third SRM is being made to calibrate concrete. The difference between these three SRMs are the aggregates and varied particle sizes. When these SRMs are developed there are often discrepancies between the experimentally determined viscosity and that predicted from the simulation. This project was focused on investigating the effects of different particle sizes and volume fractions on the rheology of fluid containing spheres suspended in a Newtonian matrix fluid. Data was gathered using a rotational rheometer, with a double spiral geometry. The viscosity was measured as a function of shear rate and the results were compared to numerical simulations. Results from this study will help provide insight into the source of discrepancy between modeling and experiment.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Zynyl Anwynn Castor		
Academic Institution: University of the District of Columbia	**Major:** Mathematics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Graduate school in Applied Mathematics	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Engineered Fire Safety Group	
NIST Research Advisor:	Randall McDermott	
Title of Talk:	Incorporation of BlenderGIS into FDS modeling workflow	

Abstract:

The Fire Dynamics Simulator (FDS) is an open source computational fluid dynamics (CFD) model of fire-driven fluid flow. NIST and its collaborators have produced validation cases to ensure that FDS produces reliable results.

FDS takes parameters from an input file. When complex geometry is needed it is convenient to make use of third-party tools to generate the input file parameters. Emanuele Gissi, a collaborator in Italy, has written an add-on to Blender (a 3D modeling/animation software) called BlenderFDS which, in conjunction with another Blender add-on called BlenderGIS (Geographic Information System), enables FDS users to build cases around terrain data easily.

For this summer, the research focused on wind flow around Askervein Hill to validate FDS for outdoor wind fields relevant for wild land fire spread modeling. Importing terrain data with BlenderGIS, building the necessary geometries for FDS using BlenderFDS, and finally exporting the FDS input file are the first steps in setting up the validation case. However, further work, such as running the model and analyzing the output is needed to complete the validation study.

BlenderFDS and BlenderGIS are significant improvements to terrain input, allowing FDS users to incorporate more complicated datasets. However, several issues remain, including details of vegetation type, soil moisture content, and ignition source data that will be required for accurate wild land fire spread modeling.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Clare Chan		
Academic Institution: Columbia University	**Major:** Civil Engineering	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Pursue a Master's degree in Civil Engineering and career as a Structural Engineer	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Inorganic Materials Group	
NIST Research Advisor:	Scott Jones	
Title of Talk:	Rheological characterization of 3-D printable cement paste	

Abstract:

As technology advances, the industry seeks an alternative to the traditional way of constructing with concrete. Additive manufacturing, or 3D printing, is promising as it provides an efficient and cost effective way to build infrastructure. Although 3D printing has been applicable in other fields for years, it is relatively new in the concrete industry, requiring a new set of standards to assess the quality of 3D prints.

To understand how printable a concrete mix is an experimental design of 16 prints is used. Each print has a different combination of five variables: water-cement ratio, high-range water-reducing admixture, nozzle diameter, print speed, and layer height. Water-cement ratio and high-range water-reducing admixture affect the composition of the mix itself, while the other three variables concern the printing process. The rheology of these concrete mixes is also studied through a parallel plate test. The parallel plate test provides data concerning the shear stress, shear rate, viscosity, yield stress, and time dependent behavior of the cementitious materials.

Through additive manufacturing, the maximum number of layers before failure and the printing window (optimal time for printing concrete) for a specific mix can be found. By comparing the data collected from the 3D prints and the rheometer, we can better understand how properties such as yield stress and plastic viscosity affect the quality of a 3D print.

By finding the link between the rheological properties and the corresponding quality of a 3D print, a criteria can be determined to help us understand the applications of 3D printing cementitious materials. This can also provide insight into which materials are preferred for larger scale additive manufacturing.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Clio Chen			
Academic Institution:	Manhattan College	**Major:**	Civil Engineering
Academic Standing (Sept. '19):	Junior		
Future Plans (School/Career):	Pursue M.S. in Construction Engineering & Management		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Structures Group		
NIST Research Advisor:	Travis Thonstad		
Title of Talk:	Development of Adaptable Concrete Structures Using Non-Newtonian Fluids		

Abstract:

In reinforced concrete structures, forces are transferred between steel rebar and concrete through bond at their interface, which leads to a uniform response in terms of stiffness, strength, and ductility. While this behavior is advantageous when designing primarily for a single loading scenario, structural performance may be hindered when considering the multitude of loading scenarios a structure can experience during its lifetime. As an alternative, adaptable structures are capable of adjusting their stiffness and strength in reaction to the applied loading. One potential method is to modify the bond behavior between the rebar and concrete. This "conditional" bonding of reinforcement can be achieved by incorporating non-Newtonian fluids, whose viscosity depends on the shear rate, to passively adjust the response of select components within the structure. Although non-Newtonian fluid applications exist in a number of fields, their use remains relatively unexplored in civil engineering.

To explore the feasibility of using non-Newtonian fluids in reinforced concrete structures, elastomers, elastomer foams, and industrial clays were investigated to characterize their constructability, workability, absorption, chemical compatibility, and mechanical properties. Experimental tests of the materials in compression and the bond between the materials and rebar were conducted. The bond specimens consisted of a length of rebar embedded in the candidate material cast into a steel corrugated duct centered in a concrete cylinder. The results were then analyzed to determine the effect of several key factors on bond performance, including surface treatments, geometric factors, and material properties. The results of these experiments will serve as a basis for future studies on adaptable concrete structures and will inform upcoming tests investigating the effect of strain rate on the cyclic properties of conditional bonding strategies incorporating non-Newtonian fluids.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Alexander Conrad			
Academic Institution:	University of Maryland University College	**Major:**	Psychology
Academic Standing (Sept. '19):	Graduated May 2019, Bachelors of Science		
Future Plans (School/Career):	I plan to have a career in Developmental Psychology.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group		
NIST Research Advisor:	Ronald Lankone		
Title of Talk:	Investigating PVC Reciprocity Throughout SPHERE Irradiance		

Abstract:

Laboratory-based accelerated weathering of commercially available products and engineered materials has been utilized in many a study to investigate the impact of exposure to the natural world on such products and materials. Accelerated weathering is often used in place of natural weathering because it significantly increases the rate of sample degradation. One such strategy towards accelerated sample degradation is the NIST SPHERE (Simulated Photodegradation via High Energy Radiant Exposure), which exposes samples to elevated ultra-violet intensities at precisely controlled temperatures and levels of relative humidity. In the present study, the NIST SPHERE was used to investigate the photodegradation of polyvinyl chloride (PVC) home siding. Since its introduction during the 1950's in Levittown, Pennsylvania, PVC siding has emerged as a leading home siding material, but the long-term performance and durability of modern PVC formulations is largely unknown. A point of emphasis in this study was to determine if the high radiant flux of the SPHERE degraded PVC in the same manner as it would naturally, albeit at an accelerated rate, thus adhering to a concept known as reciprocity. Toward this end, commercially available PVC siding samples were exposed in a custom sample holder which permitted precise control over Ultraviolet intensity incident on the samples with three filters of 40%, 67%, and 90% irradiance. After increasing periods of exposure, the extent of degradation resulting from each UV intensity was characterized with ATR-FTIR and color-gloss measurements. Findings from this study will inform polyvinyl chloride degradation adherence to reciprocity, which is key to confirming that SPHERE exposure is a viable route to investigate long-term performance of PVC on an experimentally tractable time scale.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Tejas Dinesh		
Academic Institution: University of Alabama	**Major:** Environmental Engineering	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Will continue studies at grad school	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, HVAC&R Equipment Performance Group	
NIST Research Advisor:	Vance Payne	
Title of Talk:	Optimizing Heat Exchangers	

Abstract:

Heat exchangers with optimized tube configurations for their airflow patterns (via the use of a general algorithm) can result in benefits including reduced size, cost, and refrigerant charge, as well as an increase in capacity and efficiency (coefficient of performance (COP)). This project compares the performance of an airflow-optimized outdoor heat exchanger to an outdoor heat exchanger that has not been optimized. To accomplish this, the Heat Pump Environmental Chambers are employed to test the performance of a heat pump outdoor unit when connected to the optimized and standard heat exchangers for various outdoor air conditions. Performance curves of the power and cooling capacity of each configuration will be created and compared to one another to determine if there is a significant improvement due to the optimization of one of the heat exchangers.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Steven Fang		
Academic Institution: University of Maryland College Park	**Major:** Electrical Engineering	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Graduate School	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Network Control System Group	
NIST Research Advisor:	CheeYee Tang	
Title of Talk:	Industrial network interface for railroad operation simulation framework	

Abstract:

An increasing trend amongst Industrial Control Systems (ICS) is the reliance of Internet connection or the usage of a large network to communicate necessary information between multiple devices within the system. While the connecting and networking of ICS have provided significant improvements in accessibility and overall productivity, it does open up the door to potential cyber attacks. Cybersecurity measures need to be in place to protect both legacy and modern ICS from the threats of cyber attacks, however, such measures could also alter the speed and reliability of ICS communication, disrupting performance.

This project will be emulating a real-world ICS, by adding an industrial network interface to a railroad simulation framework. The industrial network selected is the Controller Area Network (CAN) module, with a Programmable Logic Controller (PLC) used as the CAN network controller. The CAN nodes will be setup on the PLC and the simulator to establish network connection. Communication protocols will be developed to exchange sensor and controller information, and the PLC will be programmed to retrieve payload information from the CAN network and communicate to the Ethernet network. This research aims to establish a hardware-in-the-loop testbed to perform research on cybersecurity measures in railroad systems. The testbed also allows network traffic to be monitored and analyzed as a series of cybersecurity measures are deployed on the system.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: June Greenstein			
Academic Institution: University of Maryland, College Park		**Major:** Chemistry	
Academic Standing (Sept. '19):	Sophomore		
Future Plans (School/Career):	I plan to obtain my bachelors degree and possibly attend graduate or law school.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group		
NIST Research Advisor:	Stephanie Watson		
Title of Talk:	Tracking Cable Degradation in Nuclear Power Plants		

Abstract:

Nuclear power plants have been in use for less than a century, and they provide 20 percent of U.S. electricity. Cables used in nuclear power plants are crucial to operational safety—cable failures have caused plant shutdowns in the past. The Nuclear Regulatory Commission (NRC) charged NIST to determine the service lives of cables used in nuclear power plants, as well as appropriate condition monitoring tests to track the degradation of in-service cables. Nuclear power plant operators can use condition monitoring tests—visual, electrical, mechanical, and chemical techniques that measure cable health—throughout the service life of a cable to ensure safe use. NIST artificially accelerates cable aging via exposure to temperature, humidity and gamma radiation in order to investigate cable response to condition monitoring tests over time. The cables are exposed to a range of temperature, humidity and gamma dose at Sandia Laboratory. Every two months, samples of the cables are taken, and a variety of tests—such as elongation at break and Fourier-transform infrared spectroscopy—are used to measure cable degradation. When this ongoing project is complete, NIST will reach conclusions on which condition monitoring tests best track cable degradation, as well as work to predict the service lives of cables used in nuclear power plants. The NRC will use these results to inform future procedures regarding cables used in nuclear power plants. This talk will outline NIST's experimental design and present preliminary results.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Daniel Hartenstine			
Academic Institution: Millersville University		**Major:** Computer Science	
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	Interning this Fall at Walt Disney World, then graduating in Spring 2020, followed by graduate school.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Systems Engineering Group		
NIST Research Advisor:	Timothy Sprock		
Title of Talk:	Creating A Data Processing Pipeline Architecture For Manufacturing Systems		

Abstract:

Modern manufacturing facilities contain many data sources, such as machine sensors, producing large amounts of raw data. While significant research effort has been put towards analyzing the collected data, there are few documented best practices on how to collect and transport data from the shop floor. However, there are many technology stacks developed by technology companies for high-transaction applications, such as social networking sites. The research goal is to reduce the barrier to adopting these tools to deploy more resilient and scalable shop floor data collection infrastructure.

The data collection architecture was implemented using: 1) Mosquitto a lightweight message broker implementing the MQTT standard (ISO 20922) that allows message publishing clients to be deployed on equipment requiring a small footprint, such as shop floor machines and other IOT devices. and 2) Apache Kafka a massively scalable message broker that enables connecting many data analytics applications and storage technologies such as MongoDB, Elasticsearch, and Cassandra. These tools were chosen due to their open-source nature, and the fact that they are considered best-in-class tools being used by high transaction applications such as Linkedin, Uber, and Spotify.

Our implementation creates a data pipeline capable of collecting MTConnect-compliant data from NIST's Smart Manufacturing Systems (SMS) testbed and storing that data in multiple databases to be used for analytics. The resulting documentation and reference implementation serve as a guideline for implementing the data collection and processing pipeline. The research shows that these tools can be applied in the manufacturing domain and will help reduce industry's risk to adopting these tools. The result is that manufacturers can more efficiently gather and store data from the shop floor and make it accessible to applications, such as scheduling systems and data analytics, that will help improve efficiency and reduce costs.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Mariam Hasan	
Academic Institution: Virginia Polytechnic Institute and State University	**Major:** Biomedical Engineering and Neuroscience
Academic Standing (Sept. '19):	Sophomore
Future Plans (School/Career):	Finish college and work in industry
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group
NIST Research Advisor:	David Goodwin
Title of Talk:	Degradation of Fiber-Reinforced Polymer (FRP) Composites Used as Building Retrofits

Abstract:

Retrofits made of strong and durable materials can help a structure survive an earthquake or surpass its initial design life of about 50 years. Fiber-Reinforced Polymer (FRP) composites retrofits have become more prevalent in infrastructure applications in the past 20 years because they have a low cost, are lightweight, and can be easily and quickly applied to tight spaces within existing structures, unlike traditional steel retrofits. FRP composites are available in two forms, carbon and glass, and can be applied as a woven fabric sheet by applying liquid epoxy and allowing it to cure within the fabric and to the underlying substrate.

Though the popularity of FRP retrofits has increased, it is still unclear exactly how long FRP retrofits will improve the performance of their structure. Furthermore, there are still many inspectors that lack experience with assessing FRP composite conditions in the field.

In 2018, a team of NIST researchers was deployed to Anchorage, Alaska to investigate the effects of the 7.0 magnitude earthquake on its infrastructure and local community. During this deployment, FRP composites were found to fare well during the earthquake but there were some signs of FRP degradation in the exterior samples that had been exposed to subarctic climates for 10 to 15 years. For this reason, FRP/concrete bonded samples were extracted from the interior and exterior of various buildings in Anchorage, Alaska and compared using chemical measurements, thermal measurements, and microscopy. Measurements such as Raman microscopy, attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR), micro ATR-FTIR Spectroscopy, thermogravimetric analysis (TGA), and scanning electron microscopy were used on FRP composite/concrete bonded samples to investigate the degradation of both the concrete-FRP composite interface and the bulk FRP composite material outdoors.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Lindsay Hutton	
Academic Institution: Purdue University	**Major:** Environmental and Ecological Engineering
Academic Standing (Sept. '19):	Sophomore
Future Plans (School/Career):	Pursue a career in Environmental Engineering
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Div., Inorganic Materials & Polymeric Materials Group
NIST Research Advisor:	Scott Jones and David Goodwin
Title of Talk:	Polymer Modified Cements for 3-D Printing Applications

Abstract:

Additive Manufacturing has the capacity to advance current methods of building structures. The idea holds a lot of promise but faces two obstacles: speed of building and need for reinforcement. An approach to tackle these both is to mix a fast-setting polymer into cement paste, which could potentially improve buildability by more rapidly increasing material shear strength and provide more ductility in the material. These properties would allow for more material to be added more quickly, as well as decrease or eliminate the need for reinforcement. This study focused on the implications of adding a polymer to cementitious materials to 1) determine the early age properties of the modified cement (i.e., setting time, shear strength, hydration time) before hardening and 2) evaluate the late age mechanical properties of the modified cement after hardening. Epoxy, a thermoset polymer that is known to strongly interact with concrete, was the polymer type added to cement in the study. Cement samples were prepared with a 10 % mass loading of three different epoxies and cement controls were prepared without added epoxy. For early age properties, time of setting was determined using VICAT measurements, and the flow properties were determined using rheometric techniques. Mechanical properties of the samples were characterized using three-point flexural, compression, and custom-designed tensile tests for cement samples. Calorimetry was also used to characterize the hydration kinetics of the cement. The epoxy that showed the best early and late age properties was selected to be tested at mass loadings of 7.5 %, 10 %, and 20 % to determine the most successful ratio of epoxy to cement paste.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

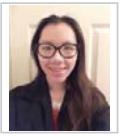
Name: Jared Kaplan			
Academic Institution:	University of Maryland, College Park	**Major:**	Mechanical Engineering
Academic Standing (Sept. '19):	Junior		
Future Plans (School/Career):	Finish my undergraduate degree and enter the work force for a few years before attending graduate school.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Cognition and Collaboration Systems Group		
NIST Research Advisor:	Brian Weiss		
Title of Talk:	Health Degradation Assessment for Robotic Manufacturing		

Abstract:

Manufacturing processes have become increasingly sophisticated where many manufacturers have turned to robotics to perform many of these complex tasks to enable and enhance production. Maintenance is an integral part of a successful and sustainable robotic system, especially within manufacturing. Maintenance can be very costly, leading some manufacturers to unnecessarily spend resources (i.e., time, money) to maintain their equipment. Billions of dollars are lost each year due to unexpected equipment maintenance.

To reduce maintenance costs, manufacturers are exploring how they can assess the health of their robotic manufacturing equipment to optimize their maintenance schedules. As part of the NIST Smart Manufacturing research, the Prognostics and Health Management for Reliable Operations in Smart Manufacturing project aims to develop methods to assess the health of a robot work cell; the work cell includes the robot along with necessary components to enable the work cell's process including end effectors, sensors, fixtures, controllers, and supporting automation (e.g., conveyors).

A test method, along with a companion sensor, has been developed to assess the health degradation of a robot work cell. Although the test method and sensor are operational, further verification testing is required. The project focuses on testing the companion sensor using a multi-axis linear stage that will check process success at points around the sensor. The goal is to automate this testing process, as testing hundreds of points manually becomes tedious. Using Matlab and an oscilloscope, the process has been automated by creating an algorithm that can pick points from a list (e.g., randomly, horizontally, or vertically) and integrating the sensor feedback into Matlab through the oscilloscope. The algorithm automatically tests sensor response at each point once the user selects their preferred test approach. The results are then stored in Matlab and exported to excel where they can be formatted into grids and analyzed to draw conclusions about the test method and the sensor.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Nina Lau			
Academic Institution:	University of Maryland Baltimore County	**Major:**	Chemical Engineering
Academic Standing (Sept. '19):	Sophomore		
Future Plans (School/Career):	Aiming for a career in industry		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group		
NIST Research Advisor:	Deborah Jacobs		
Title of Talk:	Accelerated Weathering of Polyester Using Integrating Sphere Technology		

Abstract:

Accelerated weathering devices provide a faster way to carry out service life prediction than outdoor tests. This is because factors that cause chemical degradation such as UV exposure are several times stronger inside the device than outdoors However, current accelerated weathering technologies are often unreliable and inaccurate due to uneven distribution of heat and UV light. The Simulated Photodegradation via High-Energy Radiant Exposure (SPHERE) device is based on integrating sphere technology which allows uniform light scattering inside the SPHERE thus providing more accurate and repeatable tests.

In this study, samples of polyester were exposed to either the SPHERE or to outdoor conditions. These samples were intermittently tested for chemical degradation via ultraviolet–visible spectroscopy and fourier-transform infrared spectroscopy, each measuring in the ultraviolet and infrared regions respectively.

The resulting data was compiled and shows spectrum-wide changes in absorbence as well as tracking changes at specific wavelengths. These changes can be attributed to changes in the chemistry of the sample. Upon comparing the degradation data of the SPHERE samples to the outdoor ones, the SPHERE's ability to reproduce the natural weathering of polyester will be assessed.

If the SPHERE is able to degrade samples the same way they degrade outdoors, this will be a significant step towards establishing integrated sphere devices as a better alternative to the outdated technologies used currently. It will allow for more accurate service life prediction and help manufacturers produce better, longer-lasting products.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Adam Lenker		
Academic Institution: Messiah College	**Major:** Cybersecurity	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	NIST (Cybersecurity Analyst)	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, National Fire Research Laboratory Group	
NIST Research Advisor:	Matthew Hoehler	
Title of Talk:	Web-Based Data Augmentation of 360-Degree Video for Fire Research	

Abstract:

360-degree video is a unique tool to understand fire behavior in experimental fire research. A new camera enclosure developed at the National Institute of Standards and Technology (NIST) allows viewers to watch fire growth and decay from the middle of large fires. In parallel to this 360-degree video footage, large amounts of sensor data are recorded during fire experiments. The purpose of this project is to develop web-based software to integrate data directly into 360-degree video.

This project uses a web-based augmented reality (AR) technologies including WebAR and WebGL to integrate the data into the videos for viewing on either a web browser or head mounted display (HMD) virtual reality headset. The software platform is A-Frame, which allows development of web-based virtual reality programs. The coding will be done on a related site named Glitch. The primary computer programming languages used are HTML (to display the video and its related components) and JavaScript (to give each program element its intended function).

The first objective is to create the required video and timing controls for use in a web-based 360-degree environment. In addition, the viewer needs to be able to zoom in and out. Data will be displayed at interactive 'hotspots', which the viewer can select or deselected as the video plays. With this video, anyone can access the calculations by clicking on the hotspots at any point, which brings up the changing data in real time as the video plays. That way, the viewer can easily access this data without spending the large amounts of time to understand the experiment making the data more accessible to stakeholders.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Ian Mackey		
Academic Institution: Cornell University	**Major:** Electrical & Computer Engineering	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Finish my undergraduate degree, and pursue graduate school	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Information Modeling and Testing Group	
NIST Research Advisor:	Yan Lu	
Title of Talk:	HDF5 and DREAM.3D Applications for Additive Manufacturing	

Abstract:

Additive Manufacturing (AM) allows a higher degree of freedom in producing organic shapes and complex internal features at the cost of low consistency of the part quality between runs and from machine to machine. To resolve this lack of quality control, big data is generated before, throughout, and after the part's creation to help monitor and qualify the part, and allow for failure analysis. Data consists of CAD (computer aided design) models, high sampling rate time series control and sensor data, 2D in-situ and ex-situ images, as well as the meta information associated with the machine control and measurement device configurations. This project evaluated how a hierarchical data format (i.e., HDF5) and a data analysis tool (DREAM.3D) could be used to organize and analyze the AM big data.

AM data management lacks a proper way to contextualize or tag the data generated through AM product development life cycle, which is necessary for data sharing and data analytics. Without a proper temporal and spatial registration, the large amount of in-situ melt pool monitoring images cannot be used for process anomaly detection or part defect prediction, neither can they support part qualification or material process-structure-property relationship identification. HDF5 lends itself to represent this kind of data, allowing the user to tag data directly. It can efficiently capture both the data and meta information and store them in a single file easily sharable between different computers and operating systems. DREAM.3D, an open source software, manages material micro structure data based on HDF5 data format. DREAM.3D consists of data analysis tools (Filters) that allow for the construction of customized work flows (Pipelines) to analyze data. It allows for an easy shift between managing and analyzing the data generated in AM processes. The usefulness of HDF5 and Dream.3D for AM data management is demonstrated through a case study of importing a set of AM melt pool monitoring data from an existing AM material database and performing a deep learning for melt pool classification.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Riley MacLaren		
Academic Institution: Montgomery College	**Major:** Fire Protection Engineering	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Get my Associates degree in Fire Protection engineering in 2020 then obtain my Bachelors in FPE (2022). Work as a PREP student in the Fire Research Division while going to school.	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials & Structural Systems Division, Structures group	
NIST Research Advisor:	Jonathan Weigand and Travis Thonstad	
Title of Talk:	Corrosive Degradation in Concrete Infrastructure with Low-Carbon Steel and Nitinol	

Abstract:

Today, low-alloy steel deformed bars (rebar) are used to reinforce concrete structures because of their strength and durability. During an earthquake, the steel rebar deforms plastically to dissipate energy and protect the occupants of the structure. This behavior leads to acceptable performance in terms of safety. However, it has the potential to lead to large residual displacements following a seismic event. New, high-performance bridge and building systems have been developed to incorporate shape memory alloy (SMA) bars within critical regions of the structure. These bars are super elastic and will return to their original shape after being deformed, which is ideal for structures after an earthquake. The most common SMA investigated for use in civil infrastructure is Nitinol. Nitinol offers many advantages over rebar, such as an increased resistance to corrosion, however its high cost means it can only be used in critical areas for re-centering capability and performance. For the rest of the structure, rebar is used and coupled to the Nitinol to provide continuity of loads throughout the structure. This coupling leads to the potential for galvanic corrosion between the two metals, which can be worsened by favorable conditions (e.g., chloride penetration from the use of deicing salts).

To evaluate the potential and impact of galvanic corrosion between Nitinol and rebar, two experiments were conducted under different conditions. Electrochemical cells, consisting of a Nitinol bar electrically connected to a rebar in simulated concrete pore solution, to directly measure the galvanic current between the two metals. Mechanical testing of corroded, coupled rebar-Nitinol specimens was also performed, to evaluate the performance of the coupler connections under different corrosion levels. To simulate years of corrosion, these specimens were accelerated by running an impressed current through the bars. This test series lays the groundwork for developing future studies to determine the influence of galvanic corrosion caused by SMAs on structural performance, develop prevention and remediation strategies, and develop design guidance to ensure durability in civil structures that incorporate SMA bars.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Steven Mallia		
Academic Institution: Purdue University	**Major:** Virtual Product Integration	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Lead a Design Team or Coordinate PLM and Design standards for a Team	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group	
NIST Research Advisor:	Guodong Shao	
Title of Talk:	A case study for modeling machine tool systems using standard representations	

Abstract:

A typical Computer Numerical Control (CNC) machining system consists of physical machine tools, material handling devices, control systems, cutting tools, and fixtures. It is challenging to accurately and efficiently evaluate the machining capabilities of machine tools with complex kinematics because of various proprietary formats of different machine component models. This dilemma can be resolved using a digital twin of the fully assembled machining tool system in a neutral format such as the STEP standard that can be easily recognized and accepted by all CAx tools. Machine models in standard formats will facilitate the reuse of machine tool information, models in neutral file formats avoid the remodeling and reconfiguring of this information multiple times for different scenarios. In this project, a case study is performed to demonstrate the standard representation of a machining system including both machine geometric and kinematics information. The machine model is in PTC Creo format. An application is developed to extract the kinematic assembly information from the machine model and convert both geometric and kinematics information into the STEP format. This standard-based machine system model can be easily imported to another CAx tool.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Anisa Moore	
Academic Institution: North Carolina A & T State University	**Major:** Chemical Engineering
Academic Standing (Sept. '19):	Senior
Future Plans (School/Career):	Graduate from A&T and work in my field before going back to school to receive my Master's degree
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Inorganic Materials Group
NIST Research Advisor:	Lakesha Perry
Title of Talk:	Hydration Reactions in Micro-structures

Abstract:

When it comes to the most used materials in construction, portland cement is at the top of the list. However, for as much as we use cement we do not fully understand it. Specifically, how to precisely predict the interactions between water and the micro-structures in cement. Portland cement is the product of crushed cement clinkers which have four main phases. Each cement phase has a specific role in the hydration process, for example alite (calcium silicate) is very reactive in the presence of water and is responsible for setting and development of "early" strength in cement. This project focuses on calcium hydroxide which is produced primarily from the hydration of alite. The purpose is to develop and refine a procedure to accurately and reliably measure the rate of dissolution. We will use this information to increase our understanding of the interactions between solid components that are found in cementitious materials. The methods used for characterization of these reactions were thermogravimetric analysis (TGA) and inductively coupled plasma optical emission spectroscopy (ICP-OES). Data from a differential scanning calorimetry (DSC) and a scanning electron microscopy (SEM) were also used for characterization. The utilization of bulk stirred reactors aided with the dissolution of the calcium hydroxide. However, the dissolution process is challenging to execute because calcium hydroxide carbonates very easily and quite quickly when it is exposed to air. To help with this process and slow down carbonation, a new reactor was developed using 3D printing. The new reactor now has a filter attached to the side which allows the solution to be pumped out. Subsequently, the reactor can now stay sealed preventing the sample from being exposed to air while extracting solution.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Sarah Morgan	
Academic Institution: Dickinson College	**Major:** Quantitative Economics
Academic Standing (Sept. '19):	Junior
Future Plans (School/Career):	Graduate School
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Community Resilience Group
NIST Research Advisor:	Maria Dillard
Title of Talk:	Identifying Consensus Indicators and Measures to Help Assess Community Resilience

Abstract:

Across America, communities encounter threats from weather, infrastructure failures, and other hazards. These dangers become extremely problematic for communities that also have to confront disturbances to basic life functions. This project centers on the development of a Community Resilience Indicators and Measures Inventory and data analyses to help identify consensus indicators and measures. Ultimately, this effort will support the NIST resilience assessment methodology, which will provide communities with a tool to make better-informed decisions that improve resilience.

An Indicators Inventory was examined and utilized to write a codebook where new variables were created. After finalizing the codebook, a new inventory was produced showcasing quantitative and qualitative characteristics of the dataset. Next, cross tabulations and data consolidation were performed to analyze the dataset. Lastly, visualizations were created to display the results. During the presentation, methods and results will be discussed.

This work unveils common indicators and measures in the inventory. Most resilience indicators are non-compound and smaller than state that fall into other social or infrastructure. Most resilience measures are non-transferable to score, smaller than county or system component, analyzed for a building unit, and available at least nationally. Additional analyses will be shown and discussed.

These analyses will be used to get to the next step of the methodology which is to consolidate indicator and measure short names to ascertain key features in the dataset. Once the methodology is completed, it will be used by communities to measure resilience at specific points in time at the community level. Furthermore, it could possibly be used by the community to examine whether the implementations made to improve buildings and infrastructure systems allows functionality of these systems and a faster recovery time of community functions.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Laura Mundy		
Academic Institution: Towson University	**Major:** Forensic Chemistry	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Finish degree, go to graduate school, and become a professor to teach/inspire the next generation	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials & Structural Systems Division, Inorganic Materials Group	
NIST Research Advisor:	Paul Stutzman	
Title of Talk:	Establishing a New Standard Reference Portland Cement Clinker for Phase Analysis using Scanning Electron Microscopy and X-Ray Powder Diffraction	

Abstract:

Portland cement is the most common type of cement used around the world and is the basic ingredient for many products such as concrete, stucco, mortar, and certain grouts. To make Portland cement, clinkers, the nodule materials produced during the kiln phase of cement production, must be ground and mixed with other active ingredients, usually gypsum and limestone, to produce powered Portland cement. Once the cement is mixed with water, the different crystalline phases react and create hydration products which bind to the aggregates and produce the rigid structure of the final product. Due to the wide variety of uses cement has, it is essential to know not only what ingredients are in the cement but how much of each ingredient there is. As the ingredients and their ratios change, the microcrystalline structure of the cement also changes, thereby altering the state of the final product.

Through the use of scanning electron microscopy (SEM) and X-ray diffraction (XRD), the mineralogical composition of the cement is determined as well as the phase abundance, crystal size, and crystal distribution. Post data analysis allows for the different phases to be distinguished and quantified as well as individual elements. Through techniques such as Rietveld refinement and image analysis, the data gathered from these two methods can then be used to establish certified reference values and uncertainties for the mineralogical composition of the cement clinker. In this project, the results that are collected will be used to created a new NIST Portland Cement Clinker Standard Reference Material that will represent the range of textures and compositions of clinkers across North America.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Dianeliz Ortiz Martes		
Academic Institution: Univ. Ana G. Méndez - Recinto de Gurabo	**Major:** Industrial & Management Eng.	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Finish my bachelor's degree and pursue a career in operations research	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials & Structural Systems Division, Structures Group	
NIST Research Advisor:	Joseph Main	
Title of Talk:	Documenting Characteristics of Hospitals Impacted by Hurricane Maria in Puerto Rico	

Abstract:

On September 20, 2017, Hurricane Maria made landfall on Puerto Rico as a Category 4 hurricane, with sustained winds of 249.4 km/h (155 mph). Hurricane Maria caused great damage throughout the island, leaving 100% of the residents without electricity and 11,229 residents seeking refuge in storm shelters. Buildings sustained serious damage, and only seven out of about 70 hospitals were able to resume operation after the hurricane. The total cost of damages is estimated at nearly $100 billion. Motivated by these severe damages, the National Institute and Standards and Technology (NIST) has launched a multi-year study of Hurricane Maria's effects on Puerto Rico, with a focus on better understanding how buildings and infrastructure failed. The goal of this study is to develop recommendations for improved codes, standards and practices to prevent such failures in the future. The purpose of this summer research is to document key characteristics of hospitals in Puerto Rico to guide the selection of a sample of hospitals for further evaluation. Important information for the sample selection includes characteristics of the building itself, such as the building height, elevation, and date of construction, as well as information on hazard exposure, such as the flood zone, the peak wind speed, and the effect of the surrounding topography on wind speeds. This information has been collected by identifying available sources of data and using ArcGIS Pro and Google Earth. Once the sample of hospitals is established, damages and loss of function will be documented in detail. One or more of the buildings from this sample will be tested in a wind tunnel, using scale models of the building and its surroundings to evaluate the wind loads. Information from these studies will be used to develop recommendations to make communities across the United States more resilient to hurricanes and other natural hazards.

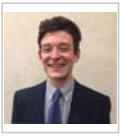
SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Sriniket Rachuri		
Academic Institution: University of Maryland	**Major:** Mechanical Engineering	
Academic Standing (Sept. '19):	2nd year (Sophomore)	
Future Plans (School/Career):	Work for a few years and attend graduate school	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, Mechanical Systems and Controls Group	
NIST Research Advisor:	Natascha Milesi-Ferretti	
Title of Talk:	Using HVAC-Cx in the Building Commissioning Process	

Abstract:

Commercial buildings account for a significant portion of U.S energy expenditures and this portion is only expected to rise. In many cases, the Heating, Ventilation, and Air Conditioning (HVAC) systems within these buildings do not operate as designed, wasting large amounts of energy and compromising occupant comfort. HVAC commissioning (Cx), which is the process of analyzing the performance of HVAC systems during or after construction, allows buildings to perform closer to their design intent, saving energy and improving occupant comfort in the long run. However, Cx is a very labor-intensive process, requiring data collection and analysis; with most buildings featuring multiple Air Handling Units (AHUs), dozens of terminal boxes, and other components, it is not practical to commission a building manually. HVAC-Cx, a software tool developed at NIST, is designed to automate portions of the Cx process using the HVAC system's own control and sensor data. Locating faults within the system, generating fault reports, presenting evidence of faults in graphs, running functional performance tests in real-time, and generating a list of possible causes are among the many features in HVAC-Cx. This project focuses on using HVAC-Cx to analyze data collected from the Performing Arts Center at Montgomery College and the Virtual Cybernetic Building Testbed (VCBT) at NIST, and to draw conclusions based off this data. HVAC-Cx will be utilized at the Performing Arts Center to locate faults within the HVAC system, identify possible causes for these faults, and recommend solutions to the operators. For one 12-day period from April 29th to May 10th, HVAC-Cx reported numerous faults from different components of the HVAC system, ranging from sensor faults to control sequence logic faults. This project uses HVAC-Cx with the VCBT to test the performance of the sequence of operations created by ASHRAE for dual duct AHUs. Confirmation of the correct implementation of the guidelines will be done by running test scripts in the VCBT.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Samuel Riddle		
Academic Institution: Virginia Tech	**Major:** Engineering Science & Mechanics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Graduate studies in Engineering Mechanics	
NIST Laboratory, Division, and Group:	Engineering Lab, Materials & Structural Systems, Polymeric Materials Group	
NIST Research Advisor:	Jae Hyun Kim	
Title of Talk:	Quantitative Visualization of Crack Formation in Polymer Backsheet Materials	

Abstract:

The mechanical properties of polymers change significantly after weathering, making them susceptible to cracking. This poses a problem for photovoltaic (PV) modules, which rely on polymer backsheets for protection from excessive heat and humidity. Microcracking in the backsheets can be a source of environmental degradation that causes a safety concern for the PV module. The ability to quantify the formation and propagation of these microcracks is an important step in understanding this problem. Two methods were employed to explore the cracking: digital image correlation (DIC) and acoustic emission (AE). The DIC system detects cracks formed in the PV backsheets by locating high strain fields. This method requires a high magnification to monitor microcrack formations and can therefore only be used to observe a small portion of the sample being tested. To compensate for this small area, AE was used to detect fracture energy released by microcracks in an entire specimen and convert it into an electrical signal. The intensity of each event can be defined by a number of descriptors including the number of threshold crossings or counts, the duration time of the event, and the peak amplitude. First, unaged samples were given shallow cuts to simulate cracking. The DIC system was able to locate the simulated cracks, validating the testing method. Accelerated weathering of a polyamide-based backsheet was then conducted using Simulated Photodegradation via High Energy Radiant Emission (SPHERE) technology at the National Institute of Standards and Technology (NIST). Samples underwent accelerated weathering for 10 days and 20 days. Tensile tests were performed for both the 10-day sample set and the 20-day sample set, while DIC and AE data were simultaneously collected to monitor microcrack formation.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Isaac Rose		
Academic Institution: University of Maryland	**Major:** Aerospace Engineering	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Pursuing B.S., will likely attend grad school following graduation	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Cognition and Collaboration Group	
NIST Research Advisor:	Helen Qiao	
Title of Talk:	High-precision Stereo Camera Calibration and Assessment	

Abstract:

Robotics is a rapidly growing component of manufacturing, and maintaining good robot health is vital for keeping up production and minimizing costs and setbacks. Stereo camera vision systems, which can measure seven degrees of accuracy for robotic arm/tool movement - x, y, z placement; roll, pitch and yaw; and time - are good for acquiring quick and accurate measurements. Every pair of images or video frames collected by the vision system can be triangulated, or transformed into a 3D reconstruction, to measure the exact location and orientation of objects in the camera frame. However, this system's accuracy depends on its calibration, which in many applications must map every pixel from the camera frame into the '3D world' within 0.1-pixel accuracy. One common challenge of stereo-camera calibrations is that the limited overlap between the two cameras' frames of view inhibits the ability to capture an array of calibration images that fill the individual camera frames, weakening the calibration. We modified a MATLAB toolkit to first use separate sets of images for individual camera calibration and then analyze shared images of a smaller checkerboard area for a more robust stereo calibration. We also explored comparing the measured relative positioning of two cameras in a stereo calibration to their real positions/orientations as a measure of single-camera calibration accuracy. In another calibration accuracy test method, we took images of a board containing three parallel lines, applied the calibration-dependent distortion model and analyzed the linearity of the lines after undistorting the images. Measuring the accuracy of our calibrations allowed us to better characterize the features of a strong calibration, such as the calibration board's position in the optical frame and camera settings like exposure and frame rate. Using feedback to improve and better characterize good calibration practices will enhance calibration consistency and vision system measurements.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: William Saar		
Academic Institution: University of Maryland	**Major:** Fire Protection Engineering	
Academic Standing (Sept. '19):	Graduate Student	
Future Plans (School/Career):	Pursue M.S. in Fire Protection Engineering at the University of Maryland	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Flammability Reduction Group	
NIST Research Advisor:	Isaac Leventon	
Title of Talk:	Pursuing Improved Solid Pyrolysis Models	

Abstract:

To more accurately predict fire growth and flame spread for a material, its thermophysical properties and the mechanisms controlling flame spread and must be measured. These mechanisms - which include thermal decomposition, production of gaseous pyrolyzate, and heat transfer (both through the material and from the flame to the material's surface) - can be measured through a series of milligram- and gram-scale experiments. Measurement data from these experiments can be analyzed to build material degradation models for which bench- and full-scale tests can provide final validation.

In this work, necessary apparatus for these experiments are constructed and run. A new gram-scale, controlled-atmosphere gasification apparatus is constructed and existing NIST gasification apparatus is refurbished. A new bench-scale flame spread apparatus is constructed and full-scale testing is performed to measure flame to surface heat flux and fire growth rate during upward flame over several polymeric materials. This work is conducted to contribute to our understanding of the mechanisms controlling flame spread over combustible solids and to the development and validation of the NIST Fire Dynamics Simulator, which is used to simulate this behavior.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Esteban Segarra Martinez		
Academic Institution: Florida Polytechnic University	**Major:** Computer Engineering	
Academic Standing (Sept. '19):	Graduate Student (Initiating PhD studies)	
Future Plans (School/Career):	Graduate School / Research	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Manipulation and Mobility Systems Group	
NIST Research Advisor:	Jeremy Marvel	
Title of Talk:	Adaptive Metrics and Performance Analysis Tool for Human-Robot Interaction	

Abstract:

Human-robot interaction(HRI) is the interactive collaboration between an operator and a robot, allowing a greater range of tasks than a single operator or robot could perform alone. Collaboration between operator and robot can utilize extensive use of human-machine interfaces(HMI) from as simple as a mouse and keyboard to virtual reality equipment and motion tracking systems. Despite the advances in the field, many existing HMI variants provide a hit-or-miss experience for HRI and no reliable method of quantifying it. As of today, there have been many different approaches using different theoretical approaches to attempt to describe an HRI experience but very few focus on directly quantifiable metrics from HRI, mainly relying on qualitative metrics instead.

In this project, we will concentrate on a single HMI interface method containing variations on the user interface(UI). The user interface will be used to trial various control schemes for the operation of different robots. Different metrics will be taken into consideration while utilizing the variations of the user interface including operator performance, task completion time, areas of user focus, and the inclusion of external sensors such as motion capture or EEG headbands.

The tool will be utilized by researchers to test and quantify the user experience of using different UI and their interactions. Key performance metrics studied from the UI will include several metrics that focus on user knowledge, amount of time spent learning and using the UI, user performance, and comparing the results against different metric-measuring standards. The tool is expected to be part of a greater study involving different HMI for HRI applications and studying their practicality and flexibility for application in manufacturing, medical care, search and rescue, and other HRI applications.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Kyle Fox Shreve		
Academic Institution: University of Maryland, College Park	**Major:** Mechanical Engineering	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Complete my undergraduate degree at UMD and pursue a career in engineering	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Production Systems Group	
NIST Research Advisor:	Gregory W. Vogl	
Title of Talk:	Squareness Testing of Machine Tool Linear Axes Based on Inertial Measurements	

Abstract:

Machine tool linear axes move the tool and/or workpiece to the desired location for cutting. Ideally, these axes are perfectly aligned and orthogonal to one another. Unfortunately, prolonged use of machine tools can cause degradation and changes to the squareness of machine tool linear axes, which decreases the quality and repeatability of part production. While there are well-established methods of measuring the squareness of these axes, these processes are time consuming and cost prohibitive. As a result, manufacturers often forgo these measures, and deviations in squareness are often unknown until part production quality has significantly decreased.

In this project, we develop a quicker and more affordable method of measuring the squareness of machine tool linear axes. Specifically, a method that makes use of an inertial measurement unit (IMU), which contains accelerometers and rate gyroscopes, to measure motion of one or more moving linear axes. The two new methods that were tested are (1) the machine tool table is moved back and forth sinusoidally at various angles relative to a nominal axis direction to calibrate the squareness of two IMU accelerometers, followed by circular motion of the IMU at one fixed angle relative to the worktable, and (2) the IMU is moved in a circular motion at various angles relative to the worktable. To ensure accuracy and repeatability for the second method, the IMU was placed on a kinematic mount that was calibrated with a custom optical polygon for knowledge of reference angles. For both methods, Fourier fits of the data are used to measure the phase differences between the X and Y signals, and these phase differences are used in least-squares formulations to solve for the squareness of the X and Y machine tool axes (via MATLAB). We hope that either method could be incorporated into a warm-up cycle of machine tools to ensure that the squareness of the linear axes is within a specified tolerance, so that deviations in squareness can be diagnosed prior to producing defective parts.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Devon Aron Luis Suarez			
Academic Institution: University of Tennessee, Knoxville		**Major:** Computer Science	
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	Pursuing a graduate degree in Computer Science at the Univ. of Tennessee, Knoxville, focusing on High Performance Computing.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Engineered Fire Safety Group		
NIST Research Advisor:	Kevin McGrattan		
Title of Talk:	Optimization for High Performance Computing		

Abstract:

The Fire Dynamics Simulator (FDS), developed and maintained by NIST, is a computational fluid dynamics (CFD) program that solves a discretized form of the Navier-Stokes equations appropriate for fire. The program requires tens or even hundreds of CPUs (central processing units) working in parallel to perform a single simulation. Developing code to properly utilize such resources is a challenge. One tool to effectively use these resources is OpenMP (Open Multi-Processing). FDS functions by dividing the simulated area into smaller cells in which conservation equations of mass, momentum, and energy are solved. Without OpenMP, FDS sequentially iterates through these cells, performing calculations for each cell in turn. With OpenMP, multiple CPUs can operate upon separate cells simultaneously, thus moving through the domain faster. Implementation is as simple as adding single lines of code to either side of the instructions in each computation. However, haphazard addition of these lines can cause instability or inaccuracy. Tools exist to better identify proper additions. For FDS, the Intel Parallel Studio suite was used. From that suite, Intel Advisor provided a list of high value targets for editing, Intel's VTune Amplifier provided a way to track the impact of edits, and Intel Inspector eased stability testing. These tools are challenging to learn, but ultimately provide an environment that greatly facilitates effective OpenMP implementation.

The documentation resulting from this work with OpenMP and accompanying tools will hasten FDS's growth moving forward. As the code is modified, it can be optimized quickly, with developers able to evaluate the consequences of their work. Currently, FDS already uses Continuous Integration (CI), a method of code management where tests are automatically run daily to ensure the stability and accuracy of a program. The analytic processes discussed here are easily merged into the FDS CI process, further increasing the efficiency of development.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Genevieve Tan			
Academic Institution: University of Maryland - College Park		**Major:** Fire Protection Engineering	
Academic Standing (Sept. '19):	Sophomore		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Flammability Reduction Group		
NIST Research Advisor:	Shonali Nazare, Rick Davis		
Title of Talk:	Assessing the Smoldering Propensity of Wood Exposed to Direct Contact Heating		

Abstract:

The ignition of spot fires due to embers presents serious risks in wildland urban interface (WUI) fires, as they contribute to unexpected fire spread in areas distant from the main fire. Lab-generated ember studies have been mostly directed to induce smoldering and/or flaming in porous plant fuels. Ignition of solid wood under radiant heating conditions has also been studied and widely reported in the literature. However, there is a lack of similar studies for direct contact heating, particularly on solid wood fuels. To understand ember ignitions of solid wood products and to eventually develop wood products with reduced ignition risk, a standard bench-scale test method must be developed to assess the smoldering behavior of solid wood. The main aim of the project is to develop a prototype tool to assess ember ignition resistance of wood using a surrogate ember ignition source.

In this project, a plate heater is used as the surrogate ignition source to simulate a pile of smoldering embers. Smoldering behavior of wood is quantified in terms of ignition time and ignition temperature. Analysis of the preliminary data will contribute to the understanding of the conditions under which solid wood smolders when heated by direct contact. Future work may include using different configurations of conductive heaters, as well as studying the effects of air flow and moisture content on the smoldering propensity of wood.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Melissa Tensa
Academic Institution:	Oregon State University
Major:	Mechanical & Manufacturing Engineering
Academic Standing (Sept. '19):	Senior
Future Plans (School/Career):	I plan to attend graduate school at Oregon State
NIST Laboratory, Division, and Group:	Engineering Laboratory, System Integration Division, Life Cycle Engineering Group
NIST Research Advisor:	William Bernstein
Title of Talk:	Integrating Environmental Life Cycle Assessment into Parametric Design Optimization

Abstract:

Decisions made in the design phase have a significant role in determining the environmental impact of a resulting product. Therefore, integrating sustainability considerations into design optimization presents an important opportunity for mitigating the overall environmental impact of a product. Such an integrated perspective requires approaches that enable designers to quantify relationships between the design parameters and the resulting environmental effects. This is a challenging task as methodologies for environmental sustainability assessment such as life cycle assessment (LCA) are poorly integrated into engineering design and optimization setups. Furthermore, streamlined approaches for computing environmental impact during the design stage often ignore manufacturing-related impacts resulting from the geometric complexity of parts. ASTM E3012 provides guidelines for formally characterizing unit manufacturing processes (UMP) through a standard modeling information model. The UMP model captures and describes manufacturing information relevant for evaluating sustainability performance. Such formal description help automate the estimation of performance metrics based on changes in design and manufacturing attributes, such as those associated with geometric dimensioning and tolerancing. The developed work flow enables designers to integrate environmental sustainability assessment into parametric design optimization problems by using the unit manufacturing process information model. This work flow auto-generates machining instructions (i.e., RS-274) that instantiates the unit manufacturing process model to conduct quick environmental evaluations. These evaluations encode more domain-specific information than the average LCA. This leads to more accurate information about the environmental impact of these products during their manufacturing stage. In addition, this approach allows for the exploration of "what-if scenarios" testing different product conditions, including manufacturing settings, such as tool sets and machining programs. We demonstrate the work flow through a case study involving the optimization of a rigid flange coupling design wherein the geometry of a part is simultaneously optimized for mechanical strength and cradle-to-gate environmental impact.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Donald Truong
Academic Institution:	University of California - San Diego
Major:	Math - Computer Science
Academic Standing (Sept. '19):	Alumni
Future Plans (School/Career):	Full-Time Software Engineer / Possibly Grad School
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, Mechanical Systems and Controls
NIST Research Advisor:	Amanda Pertzborn, Glen Glaesar
Title of Talk:	The Unknown Factors of Heating and Cooling Air

Abstract:

There is a need to generate new efficiency standards for air conditioning because cooling energy is one of the biggest components of US energy consumption. For commercial buildings, air conditioning represents a significant part of this problem as cooling energy for commercial buildings accounts for 40% of US energy usage annually, and with global temperature rising each year it is imperative to improve the heating, ventilation, and air conditioning (HVAC) controls of commercial buildings. The Intelligent Building Agents Lab (IBAL) seeks to address this problem by finding ways to lower the cost of energy by optimizing the efficiency of the control of HVAC systems in commercial buildings. Currently, the IBAL is controlled by a LabVIEW program that controls hardware typical of a commercial building air conditioner. Simultaneously, the LabVIEW program gathers and stores data from multiple sensors placed within the lab. The data collected allows us to understand the operation of equipment in the IBAL. As part of my contribution to the IBAL, my project consisted of applying Python to IBAL's existing LabVIEW program, using various simple machine learning models to better understand the operations happening within one part of the lab, and some hands on work. Amongst the challenges I encountered were organizing data, testing different machine learning models, and discovering bizarre results within the data I was given.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: David Umansky		
Academic Institution: University of Maryland, College Park	**Major:** Aerospace Engineering	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Complete undergraduate degree and work in the defense industry in R&D	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Production Systems Group	
NIST Research Advisor:	Jason Fox	
Title of Talk:	Analysis of Surface Finish in Laser Powder Bed Fusion Additive Manufacturing	

Abstract:

Additive manufacturing (AM) technology has been researched and developed for over a quarter-century and is becoming a commonplace tool in industry for research, development, and production. Rather than removing material like most other material processing machines do, AM technology builds a three-dimensional (3D) part directly from a CAD model by placing material layer on top of layer. This allows it to build very intricate and complex components that traditional manufacturing methods simply cannot accomplish. AM technology has made monumental advances over the past 25 years, but one area in which it struggles is the ability to create a smooth or consistent surface finish. Much rougher than machined parts, AM surfaces are also not well characterized due to the complex build process and resultant topographies. To address this issue, artifacts were created using laser powder bed fusion and examined using the Alicona Infinite G5 focus variation microscope. Previously, the measurement of the artifacts was done manually; aligning and imaging using the microscope, with a higher possibility of error, low repeatability, and extensive user setup time. To improve this process, a specialized mount was created to hold the artifact and, using the microscope's unique software, a program was developed to autonomously measure and record every surface on the artifact. A process that originally took longer than a week of constant supervision and adjustments, can now be performed almost completely unsupervised and significantly quicker. This work has immense implications on the field of AM because it creates consistency in the measurement routine, allowing researchers to better analyze the effects of process variables and repeatability on surface finish. Additionally, this research enables the advancement of standards for the surface finish of metal AM parts, which industry can use to improve their production strategies and part quality.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Varsha Vejalla		
Academic Institution: University of Virginia	**Major:** Statistics and Finance	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	I plan to pursue a career in data science.	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Applied Economics Office	
NIST Research Advisor:	Jennifer Helgeson	
Title of Talk:	Business Interruption and Recovery Following a Disaster	

Abstract:

Disasters affect communities in many different ways, as each component of the infrastructure is affected by and affects other components and systems. The inter-relatedness of the systems comprising a community make damage estimates difficult to measure. The loss/damage estimates that are available tend to focus on direct losses only, are at aggregated levels, and provide lagged indicators. They often fail to capture down-stream, indirect, and sustained effects, such as business interruption and an inability of businesses to maintain their capacity, which can significantly affect both the short-term and long-term stability of a regional economy.

The goal of this research is to advance the state of knowledge in the development of community resilience - defined as the ability to prepare for anticipated hazards, adapt to changing conditions, and withstand and recover rapidly from disruptions - for small- and medium-sized enterprises (SMEs). In-person surveys were conducted in Lumberton, NC, which experienced a flood from Hurricane Matthew in October 2016. Using this survey data, a model will be built to describe the impact of the flood on SMEs in Lumberton. Specifically, the goal of this modeling project is to see how endogenous and exogenous factors of an SME affected its ability to recover both 1) in the short-term, measured as the length of interruption immediately following the flood, and 2) in the long-term, measured using survey respondents' rating and description of their own SME's recovery. This analysis will inform a longitudinal recovery study of businesses in Lumberton and provide a basis for more generalized research on business recovery.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Adam Wathieu		
Academic Institution: Georgetown University	**Major:** Computer Science, Mathematics	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Graduate Studies in a Computer Science program	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Manipulation and Mobility Systems Group	
NIST Research Advisor:	Joseph Falco	
Title of Talk:	Investigating the Standardization of Work Volume for Robotic Manipulators	

Abstract:

With growing robotic hand research and industrial use, there is an increasing need to capture the individual competencies and characteristics of these complex systems under a unified framework. To date, NIST developed several robot hand performance metrics and test methods for cataloging not only the raw traits of the technology, but also task and function-level capabilities. These measures can be used to match capabilities to end-user needs as well as provide researchers and developers insight for improving their hardware and software designs. One such capability is Work Volume, a multi-faceted measure of the space in which a hand can grasp objects. Work Volume is useful for determining and comparing the payload volumes of robotic hands. The purpose of this research is to investigate how to measure Work Volume under a standard test method.

A tool called the Manipulator Work Volume Simulator is being developed using MatLab and its Robotics Toolkit to implement forward kinematic solutions. It implements Work Volume calculations to derive three relevant measures of volumetric capability: (1) polyhedron volume given the hand kinematics and joint limits, (2) maximum dimensions of primitive shaped objects (e.g., square, cylinder, sphere) that can be grasped by the hand, and (3) volumetric characteristics given a grasp type and associated joint limits. While the software incorporates a modular design to support many hand designs, initial verification is being performed using the Schunk Dexterous Hand (SDH).

Initial testing produced expected results, and algorithms for calculating the three measures of volumetric capability are being analyzed. Using the SDH is a proof of concept where future iterations of this software tool will support a variety of robotic hand designs, including under-actuated hands. The Work Volume of a hand and its metrics and test methods continues to be refined by the project team.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Zachary Werrmann		
Academic Institution: University of Kentucky	**Major:** Chemical Engineering	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Graduate School	
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 Polymeric Degradation of Solar Module Backsheets	

Abstract:

Multi-layer polymer backsheets, which act as electrical insulators and weathering protectors, are a vital component in solar panels. The long term life span of solar panels is crucial in the aim for reliability and efficiency for solar panels. Backsheets exhibit degradation from various environmental factors, such as ultraviolet (UV) light exposure, heat, and humidity . When backsheets degrade, sensitive components on the inside are left exposed to hazards, which causes a drastic shortening of the lifespan. Polyamide backsheets were exposed in various conditions in order to explore failure characteristics of the backsheets. Serving as a useful metric in providing information on the service life, the data collected in this experiment provided valuable insight about the common failure modes. In this project, the accelerated laboratory exposure was conducted using the NIST simulated weathering device, SPHERE, in which samples were exposed to UV radiation under elevated temperatures and various relative humidities. After exposure, the samples were inspected for changes in chemical, mechanical, and optical properties. Allowing the analysis of chemical changes, Attenuated total reflection - Fourier transform infrared spectroscopy (ATR-FTIR) measured the chemical spectra of the backsheets. Tensile tests, a common procedure in material testing, provided mechanical information such as tensile strength, elastic modulus, and the elongation of the material at break . Glossimetry and colorimetry supplied optical properties for the backsheets. After exposure, significant degradation was exhibited in the backsheets, especially under the more humid conditions. The experiment was useful in working towards the creation of standards in regards to solar modules.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Thomas Wrona			
Academic Institution:	University of Maryland at College Park	**Major:**	Computer Science/Math
Academic Standing (Sept. '19):	Junior		
Future Plans (School/Career):	Finish undergraduate studies, then graduate school for computer science		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Networked Control Systems		
NIST Research Advisor:	Timothy Zimmerman		
Title of Talk:	Simulation and Data Analysis for Cybersecurity on Industrial Control Systems		

Abstract:

As with everything else, Industrial Control Systems (ICSs) are becoming more and more connected to the Internet. Seeing as ICSs are critical to most industrial processes that could affect our daily lives, it is apparent that it is critical to protect ICSs from cybersecurity threats. However, most manufacturers are reluctant to install hardware or software for cybersecurity protection because of limited knowledge of the potential impact this protection may have on manufacturing process performance. The Cybersecurity for Smart Manufacturing Systems project seeks to provide the information and recommendations necessary for cybersecurity tools to be widely implemented in ICS.

Currently, in order to make such recommendations, many time-consuming tests are performed on a physical testbed at NIST. Simulation is a promising way to increase the number of tests that can be performed. The SimPy discrete-event simulation library for Python was used to develop a software simulation of the existing testbed. Validation of the simulation was performed, including tests on both the testbed and simulation where the network behavior was changed to emulate the effects of cybersecurity protection. The results of the tests were compared to determine if the developed simulation could effectively support the ongoing testbed research. Additionally, Jupyter notebooks were implemented to speed up the data computation. Results from the notebook were validated with existing reports to see if the notebooks could accurately analyze the data.

With both of these modifications to the existing testbed, significant amounts of time can be saved. Running the testbed requires an extensive amount of manual preparation, followed by an entire hour for the testbed to produce 35 parts. The simulation requires little preparation and can produce the data for 35 parts in less than 20 seconds. Similarly, the original method for data analysis consists of substantial non-automated work, while the Jupyter notebook needs no human interaction and 30 seconds to run.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Christina You			
Academic Institution:	Carnegie Mellon University	**Major:**	Computational Biology
Academic Standing (Sept. '19):	Sophomore at Carnegie Mellon University		
Future Plans (School/Career):	Pursuing a career in industry before attending graduate school		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Firefighting Technology Group		
NIST Research Advisor:	Albert Jones		
Title of Talk:	Using Neural Networks to Detect Kitchen Cooktop Pre-Ignition		

Abstract:

In the period between 2012-2016, cooking was the leading cause of reported home fires and home fire injuries as well as the second leading cause of home fire deaths according to the US Fire Administration's National Fire Incident Reporting System. Cooktops or ranges were involved in 63% of the reported home cooking fires, 86% of cooking-fire deaths, and 79% of cooking-fire injuries. Hence, we began to explore the feasibility of an external system that accurately detects hazardous conditions leading to a fire, but prior to ignition- a period we call pre-ignition- on kitchen cooktops.

Our exploration approach uses a multi-layer perceptron neural network to produce an algorithm that classifies between normal and pre-ignition conditions given multi-sensor data obtained from within the duct above a cooktop. Datapoints from dozens of ignition and normal cooking experiments conducted in a mock kitchen were used as training data. Each experiment used different types and sizes of pans as well as varying oils and foods. The signals from multiple sensors including dust, carbon monoxide, alcohol, and smoke were recorded every four seconds during the run of each experiment. A feature selection process was carried out to determine the algorithm's optimal prediction capability. We further investigated preprocessing methods to address the raw data's dependence on plume transport, to consider analysis on the rate of change of sensor values over time, and to consider any budget constraints with the types of sensors used. The ultimate model achieves an accuracy above 95%. In comparison to industrial smoke detectors which may only alarm users after ignition, the success of this algorithm could prevent the start of kitchen fires entirely while ignoring normal cooking activities and other nuisance sources.

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ITL SURF Participants

First Name	Last Name
Damien	Beecroft
Kevin	Boby
Joseph	Converse
Daniel	DeLeon
Eve	Fleisig
Linus	Ge
Roberto	Gorbea Finalet
Thomas	Hayes
Glen	Joy
Gerson	Kroiz
Matthew	Kupferschmid
Elisabeth	Landgren
Angelica	Lin
Eric	Liu
Lily	Northcutt
Shyaer	Parvez
Sydney	Pugh
Mason	Rhodes
Caleb	Robertson
Temur	Saidkhodjaev
Justin	Slud
Cameron	Smith
Peter	Stein
Henok	Tasissa
Daniel	Tokarz
Richard	Williams
Jesse	Zhu
Kevin	Zong
Kevin	Zong

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Damien Beecroft		
Academic Institution: University of Colorado, Boulder	**Major:** Applied Math and CompSci	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	I will earn a PhD in applied math and research machine learning or cryptography.	
NIST Laboratory, Division, and Group:	ITL, Computer Security Division	
NIST Research Advisor:	Kerry McKay	
Title of Talk:	Stream Learning for Min-Entropy Prediction	

Abstract:

Cryptography relies heavily on randomness to secure information. In real-world applications, important components such as keys, padding, and nonces are normally produced by a random number generator (RNG). The amount of randomness in an RNG comes from the amount of unpredictability in one of its components, called the noise source. If one can predict the outputs of a noise source, then one could potentially determine the string of numbers from the RNG and all information encrypted with its "random" numbers. For this reason, it is important that a noise source is sufficiently unpredictable.

The unpredictability of a noise source is measured in bits of min-entropy. One approach to test the min-entropy of a noise source is to use statistical tools called stream learners. Each learner analyzes a data stream searching for a specific bias. If this bias is present, the learner will predict outputs of that noise source more accurately than guessing randomly. In this project, we analyzed several stream learners offered by Massive Online Analysis (MOA) and evaluated their performance on noise sources with known entropy.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Kevin Boby		
Academic Institution: University of Maryland	**Major:** Computer Science	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Graduate school and a masters degree in computer science	
NIST Laboratory, Division, and Group:	Information Technology Lab, Software and Systems Division, Information systems group	
NIST Research Advisor:	Dr. Peter Bajcsy, Mr. Michael Majurski	
Title of Talk:	Deep Learning: Is more training data always better?	

Abstract: Deep learning, specifically Convolutional Neural Networks (CNNs), have recently enjoyed a renaissance; becoming the backbone of most computer vision tasks like image classification, object detection, and semantic segmentation, with the most used architectures being SegNet and U-Net.

Within the field of deep learning (DL), the general consensus is that more training data results in more generalizable and robust DL models. This has been shown by reporting high DL model accuracies trained on large research datasets like ImageNet. One approach to creating large research datasets is to aggregate data sets from related experiments conducted by individual principal investigators. However, the aggregation of training data sets yields to more generalizable and robust DL models only when all data sets are drawn from the same source distribution. Our work addresses two aggregation related problems: Do all aggregated data sets come from the same population? Can we identify subsets of data sets that are within the same population?

We explored the two problems in the context of binary image segmentation task of cell cultures imaged using phase contact microscopy modality. The 10 image data sets used in this study came from experiments that vary in terms of the cell line (H9, ND2.0), cell Colony size (larger, medium, small), microscope model (Zeiss1, Zeiss2), investigators (KB, GC), and additional experiment-specific handling. We created a SegNet and U-Net model using the architecture described in their debut papers and trained them using (1) each of the 10 data sets, (2) three groups of data sets aggregated based on cell colony size, and (3) one composite data set formed from all 10 sets. Each data set consists of images and reference foreground binary masks created by staining and image analyses of fluorescent images or by visual inspections of cell biologists.

By comparing the accuracies of the two DL models trained on composite versus Individual data sets, we were able to address the first problem. With additional comparisons of DL model accuracies across three groups, two principal investigators, and two cell lines, we could address the subsets of the 10 datasets that were more likely drawn from the same Population. Based on this work, we might be able to provide guidelines for disseminating DL models trained on aggregated datasets.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Joseph Converse

Academic Institution: Miami University **Major:** Physics

Academic Standing (Sept. '19): Senior

Future Plans (School/Career): Career in Research and Development

NIST Laboratory, Division, and Group: ITL, Applied and Computational Mathematics Division, Computing and Communications Theory

NIST Research Advisor: Dr. Paulina Kuo

Title of Talk: The Implementation of Side-of-Fringe Locking Techniques to Reduce the Frequency Drift of a CW Laser

Abstract:

Lasers play critical part in much of the technology we enjoy today. From basic compact disc players to research laboratories, lasers see wide-spread use and integration due to the range of scenarios in which they can be employed. While there are many useful applications for lasers right out of the box, often there are instances when a beam with a more stable frequency is required. In these situations, a common solution is to utilize side-of-fringe laser locking techniques, which, if applied successfully, can reduce laser drift from tens of megahertz to a fraction of a single megahertz. In this experiment we attempt to implement side-of-fringe laser locking through a variety of methods. We begin by generating the feedback signal with a fixed cavity that has a transmission function which is sensitive to the laser's frequency. The laser passes through this cavity and the exiting light is picked up by a photo-detector. Via the photo-detector, the light is converted to an electrical signal which is sent to connected analog equipment for processing and then fed back into the laser to lock the frequency in place. Throughout the experiment, we replace the analog equipment with a smaller STEMlab board and observe the repercussions this has on the efficacy of the fringe-locking. The results from our research facilitate more streamlined organization, especially for research laboratories and other spaces where lasers are frequently utilized.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Daniel De Leon

Academic Institution: University of Maryland, College Park **Major:** Computer Engineering

Academic Standing (Sept. '19): Sophomore

Future Plans (School/Career): Graduate school or a career in hardware/software engineering

NIST Laboratory, Division, and Group: ITL, Applied and Computational Mathematics, Mathematical Analysis & Modeling

NIST Research Advisor: Anthony Kearsley

Title of Talk: Fractals derived from constrained optimization techniques using Newton's Method

Abstract:

Computing extrema of functions is an important problem within the field of optimization, and can be achieved using Newton's Method, a popular and iterative process for smooth functions. Functions can exhibit one, two, or even more extrema, and Newton's Method will converge to one of these extrema based on the starting point. A method known as the "line search" is employed to help Newton's Method reach a minimum, as it ensures that each iterative step has a sufficient decrease in the function value. When applying Newton's Method to the solutions of a function with complex variables, a fractal pattern known as the Julia set is observed after graphing a plane with different starting points. The convergence of these starting points is colored based on which of the solutions was reached. The primary goal of this project was to increase the likelihood of reaching a global minimum through a domain expansion procedure that utilizes two starting points. This is implemented using a "penalty method" that forces these two points to collapse into a desirable minimum. First invented by Professor William Symes, this method has been explored by Gockenbach as well as Gockenbach and Kearsley for applications in geoseismic inversion and chemical dynamics, all of which involved unconstrained minimization problems. Although this project involves far simpler problems of smaller sizes, it dives into constrained problems for the first time. After exploring this method with different constrained functions, fractal-like patterns were often observed, and the global minimum was a solution more often than the local minima, as expected. Problem formulation played a significant role in the convergence patterns observed, and certain constraint conditions were able to increase the likelihood of reaching a global minimum even further.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Eve Fleisig

Academic Institution: Princeton University | **Major:** Computer Science

Academic Standing (Sept. '19): Junior

Future Plans (School/Career): Graduate school and research/academia in computer science

NIST Laboratory, Division, and Group: Information Technology Laboratory, Information Technology Laboratory Office

NIST Research Advisor: Martin Herman, Gunay Dogan

Title of Talk: A GUI for Evaluation of Distance Metrics on Heterogeneous Data Sets

Abstract:

Fields as diverse as crime scene forensics, cell imaging, text retrieval, recognizing objects in pictures, and training neural networks all require reliable methods of classifying, clustering, and differentiating data. These tasks fundamentally depend on comparison metrics that measure the similarity of items. For example, matching a crime scene fingerprint to a suspect's fingerprint in a database might require finding the similarity between their images, boundary curves, or points of interest. Testing these similarity metrics requires the use of statistical analyses as well as a researcher's understanding of whether a metric correlates with human perception. However, most existing methods for evaluating similarity metrics are not linked to the original data, making it difficult for researchers to understand the relationship between individual items and the overall performance of their metrics.

My project was to create a Python package that provides an accessible graphical user interface for the development and evaluation of similarity metrics. Researchers working on image classification or segmentation, training and testing models, or seeking to demonstrate the effectiveness of a complex algorithm to an outside audience can explore the results of their comparison metrics while seamlessly viewing individual data points of interest. The interface links individual data items and their associated images, spectral curves, feature vectors, or other data files with various types of analyses, such as clustering, multi-dimensional scaling, and retrieval performance analyses (e.g., ROC curves) based on the metrics, as well as generating improved metrics by fusing existing ones using support vector machines. The interface aims to help users develop and evaluate models, metrics, and algorithms by enabling them to understand the numbers as well as the data behind them.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Linus Ge

Academic Institution: University of Rochester | **Major:** Mathematics

Academic Standing (Sept. '19): Junior

Future Plans (School/Career): Most likely graduate school.

NIST Laboratory, Division, and Group: Information and Technology Laboratory, Applied and Computational Mathematics Division, Mathematical Software Group

NIST Research Advisor: Howard Cohl

Title of Talk: On generating functions for q-inverse polynomials in the q-Askey scheme.

Abstract:

An orthogonal polynomial sequence is a family of polynomials that are pairwise orthogonal under some inner product. In the case of mathematical functions, the inner product is the integral of the product of the two functions over a discrete or continuous set. Orthogonal polynomials have numerous applications to engineering and physics, commonly as solutions to special differential equations. The field of q-calculus (sometimes called calculus without limits) utilizes a complex variable q and becomes ordinary calculus in the limit as q tends to 1. In q-calculus, the symmetric orthogonal polynomials organized under the q-Askey scheme are the Askey-Wilson polynomials (four independent parameters), the continuous dual q-Hahn polynomials (3 independent parameters), the Al-Salam-Chihara polynomials (two independent parameters), and the continuous big q-Hermite polynomials (one independent parameter, symmetric in a limiting sense). These polynomials are complex valued, defined in terms of basic hypergeometric series, and usually have their parameters values taken inside the punctured unit disk. We computed the basic hypergeometric representations of the corresponding q-inverse symmetric polynomials, whose parameters are taken outside the punctured unit disk. Using the basic hypergeometric representations for the regular and q-inverse symmetric polynomials, we then compared these representations to derive interesting basic hypergeometric transformation identities. We also pursued a study on how to derive generating functions and connection relations for the regular and q-inverse symmetric polynomials. In the last part of the project, we computed several generalized generating functions by combining connection relations and generating functions for these polynomials.

This talk will begin with an introduction which will include a description of our notation and some of the properties of the regular q-symmetric polynomials. This will be followed by a presentation of our main results, namely the q-inverse symmetric polynomial representations, basic hypergeometric

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Roberto Rafael Gorbea Finalet		
Academic Institution: University of Puerto Rico Rio Piedras	**Major:** Physics/Mathematics	
Academic Standing (Sept. '19):	Begining 1st semester of Masters Progam in Applied Math	
Future Plans (School/Career):	Finish Masters Program and then continue to PhD in Math or Physics	
NIST Laboratory, Division, and Group:	ITL, Applied & Computational Mathematics, Computing & Communications Theory	
NIST Research Advisor:	Dr. Lucas Brady	
Title of Talk:	Testing Quantum-Inspired Classical Algorithms	

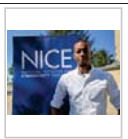
Abstract:

Quantum computers use superposition and entanglement to perform certain tasks more efficiently than classical computers. However, the physical realization of quantum computers is still under development, and thus very cost intensive. Therefore, it behooves us to consider whether or not a quantum algorithm is truly advantageous, or if there exists a classical algorithm, not yet created, that is as efficient. Quantum algorithms have helped answer this question, by giving insights that have led to the development of so-called Quantum-Inspired classical algorithms.

One Quantum-Inspired classical algorithm is Path Integral Quantum Monte Carlo (PIQMC). Quantum Path Integrals map a quantum system onto a larger classical system in d+1 dimensions. We then can calculate a minimum energy, that encodes the solution to some optimization problem, with a Monte Carlo Technique. PIQMC either directly simulates or pulls inspiration, without directly simulating the quantum dynamics, from the following quantum algorithms respectively:

1)(Quantum Adiabatic Optimization) Determines the minimum of a cost-function by slowly evolving a quantum system in some known ground state to another configuration where the new ground state encodes the solution to an optimization problem.
2)(Quantum Approximate Optimization Algorithm) Determines the minimum of a cost-function with a hybrid of 'bang-bang' alternative control schedule of unitary gates and classical preprocessing.

PIQMC when applied to (1) has been shown to have success rates correlated with (1) for solving some problems. We create a PIQMC algorithm inspired by (2). We then implement both PIQMCs to solve Max-Cut on some graphs. We compare the performance of these algorithms when applied to different types of graphs of varying size. Specifically, we plot the approximation ratio vs. number of Monte Carlo steps for each algorithm applied to graphs of varying topologies. We also study the stopping criterion of the Monte Carlo methods for future analysis of the algorithm's performance.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Thomas L. Hayes		
Academic Institution: University of North Georgia	**Major:** Information Systems	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Graduate school/Career in Cybersecurity	
NIST Laboratory, Division, and Group:	ITL, Applied Cybersecurity, National Initiative for Cybersecurity Education	
NIST Research Advisor:	Danielle Santos	
Title of Talk:	Measuring Public Awareness of Cybersecurity Careers	

Abstract:

There is a severe global shortage of cybersecurity professionals that is underscored by the frequent occurrence of massive data breaches and ransomware attacks that cost millions and sometimes billions of dollars in damage to governments and businesses of all sizes (Baker et al., 2011; Mansfield-Devine, 2016). Increasing public awareness of careers in cybersecurity is a crucial part of alleviating the shortage of cybersecurity professionals. This talk explains the urgency of the shortage of cybersecurity professionals and examines current levels of public awareness of cybersecurity careers.

At the moment, there is no data available that measures the public's basic knowledge of cybersecurity careers. To determine this baseline, a survey will be conducted, and the data analyzed. Measuring public awareness of cybersecurity careers will help organizations develop more effective strategies in alleviating the shortage of cybersecurity professionals.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Glen Joy
Academic Institution:	University of Maryland, College Park
Major:	Computer Science and Criminology & Crimina
Academic Standing (Sept. '19):	Sophomore
Future Plans (School/Career):	Seeking to pursue a Master's in Cybersecurity Engineering with the desire of working for the federal government.
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied Cybersecurity Division, National Cybersecurity Center of Excellence Group
NIST Research Advisor:	James McCarthy
Title of Talk:	Securing the Energy Sector through Standards-Based Cybersecurity Architectures

Abstract:

The energy sector is one of the nation's 16 critical infrastructures as outlined by the Department of Homeland Security. Industrial control systems (ICS), which are systems used within the energy sector to facilitate various industrial processes, present a significant portion of such critical infrastructure. ICS assets are growing in communication abilities and creating what is known as the Industrial Internet of Things (IIoT) - the vast interconnectedness of sensors, machinery, vehicles and other assets working together in industrial environments. Additionally the growing use of distributed energy resources (DER's), such as residential solar applications and wind turbines, alongside these assets create increased avenues of information exchanges. These assets then become key targets for cyber-attacks, potentially resulting in disruptions to the power grid and other industrial operations. ICS malware prevention and data integrity assurance for IIoT assets as well as asset management capabilities are therefore paramount in ensuring secure operation of energy sector assets. The following describes two cybersecurity projects to provide adaptable architecture solutions to address these problems. The first addresses data integrity and ICS malware challenges for IIoT assets. The second tackles enhancing asset management capabilities with monitoring and security features, primarily through the creation of an automated asset inventory. The end product of these projects will be two NIST SP-1800 series documents, known as practice guides, for industry to understand the problems at hand and our developed reference solutions. The solutions aim to be standards-based, modular, adaptable, and repeatable.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Gerson Kroiz
Academic Institution:	University of Maryland, Baltimore County
Major:	Mathematics & Computer Science
Academic Standing (Sept. '19):	Sophmore
Future Plans (School/Career):	Pursuing a PhD in applied mathematics
NIST Laboratory, Division, and Group:	ITL, Software and Systems Division, Information Systems Group
NIST Research Advisor:	Dr. Timothy Blattner
Title of Talk:	Exploiting Coarse-Grained Parallelism in Numerical Linear Algebra Routines

Abstract:

As scientific computations continue to increase in size and complexity, the need for optimization increases. This research investigates the optimization of linear algebra routines on matrices through coarse-grain parallelism, a method of splitting a program into large subtasks computed simultaneously. To achieve this coarse-grain parallelism, we use block decomposition, a representation of a matrix through several subregions, to produce partially solved blocks that can be sent to the next stage of computation while the remaining blocks are still in computation. Using Hedgehog, an API constructed to represent algorithms as hybrid pipeline workflows using hybrid task graphs, we developed a numerical linear algebra library including implementations of matrix multiplication and LU decomposition with and without partial pivoting. These implementations, represented as graphs, are composed of tasks and state-managers inherited from Hedgehog. Tasks perform operations on the blocks while the state-managers keep track of the block's state in the calculation.

This library exploits a new depth of coarse-grain parallelism not present in popular linear algebra libraries. In addition to using blocks of matrices within the computation, the library allows for the production of results in a block-like fashion while the remainder of the matrix is amidst computation. This design benefits a graph that consists of multiple linear algebra routines as a block's results from one routine can be used immediately in the next routine without waiting for the solution of the remaining blocks of the matrix. Early comparisons with the OpenBLAS library show comparable performance for solving large dense matrices. After further development of the Hedgehog Matrix Block Library (HMBLib), more thorough studies can show the impact this implementation of block decomposition on linear algebra routines has on performance.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Matthew Kupferschmid		
Academic Institution: Washington University in St Louis	**Major:** Mathematics	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	I plan on continuing to work in the field of statistics and maybe go to graduate school	
NIST Laboratory, Division, and Group:	ITL, Statistical Engineering Division, Statistical Design, Analysis & Modeling Group	
NIST Research Advisor:	John Lu	
Title of Talk:	Saving Lives with Cooktop Sensors	

Abstract:

Cooktop fires are very destructive in our society. Nearly 50% of reported home fires involve cooking equipment. With this in mind it is important to identify technology that can make our kitchens safer. New regulations require cooking equipment to have an installed sensor that will identify when a fire will occur and shutoff the stove. Even with these new regulations that prevent possible tragedy there are still over large amounts of older stoves across the United States that do not have these installed. This creates the need for a retroactively fit technology that can turn the stove off if it senses a possible fire.

82 different trials were conducted with various pans, oils, and foods that produced different outcomes from 20 different sensors. We used R programming to perform data analysis on the data gathered and figure out what sensors were needed for the possible new technology to perform best.

Using R, we were able to create time series graphs, logistical models, and receiver operating character (roc) curves. We then gathered additional knowledge when we looked into the area under the roc curves, the rate of change of various sensors, and the maximum values each sensor reached before a fire. While this research can continuously be done, I believe that the research that I and others have done this summer can work towards creating a usable device that can save lives.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Elisabeth Landgren		
Academic Institution: Macalester College	**Major:** Computer Science	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Pursuing a career in computer science.	
NIST Laboratory, Division, and Group:	ITL, ACMD, High Performance Computing and Visualization Group	
NIST Research Advisor:	Steven Satterfield	
Title of Talk:	Quantum Dots and Virtual Reality: The Pursuit of Intuitive Data Realizations	

Abstract:

The National Institute of Standards and Technology (NIST) has been developing a virtual measurement and analysis laboratory in a 3D immersive virtual environment using a Cave Automatic Virtual Environment (CAVE) hardware configuration and a High End Visualization (HEV) software system for over 20 years. The CAVE at NIST currently consists of high quality projections onto three screens on the floor and walls that create tracking 3D images and animations using infrared tracking technology. Interdisciplinary researchers utilize this technology both for the purpose of understanding their data from the inside out as well as for creating customizable visualizations they can use to gain visibility and present their findings. Although the HEV system is designed to create applications usable on a personal desktop as well as the CAVE, the CAVE is a unique tool that allows researchers to take a step inside their world of data and get a different perspective of what is going on.

In the CAVE, the user experience is fairly intuitive, as the 3D virtual world mimics the real 3D world visually. Historically, however, the navigational elements of the CAVE have been complex and required fairly extensive knowledge of the software to be operated smoothly. The focus of this project has been to put the user back in control by adding more intuitive commands to be used in the place of input and control operations without deprecating existing advanced operations used by more experienced users. The final product is a quantum dot visualizer application to showcase the functionality of the new navigational tools. This prototype will serve as an example for how more user friendly interfaces could be implemented into the larger HEV structure to aid researchers in more autonomous data visualization.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Angelica Lin			
Academic Institution:	College of William & Mary	**Major:**	Applied Mathematics
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied & Computational Mathematics Division, Mathematical Analysis & Modeling Group		
NIST Research Advisor:	Anthony Kearsley		
Title of Talk:	Applied Chemometric Methods for Monoclonal Antibody Classification		

Abstract:

Monoclonal antibodies (mAbs) are biologic drugs designed to target a specific disease in the body, such as cancer. They can be used alone to directly destroy harmful cells, or engineered to deliver medication for radiation therapy or chemotherapy. Unfortunately, the cost to administer these drugs is currently prohibitive. However, pharmaceutical companies are developing generic alternatives to mAbs called biosimilars. By introducing biosimilars to the pharmaceutical market, especially for those medications that have been in use longer than patent protection duration, research competition among companies will increase and ultimately lower the costs of mAbs.

An important attribute of biologic drugs is higher order structure, which includes secondary, tertiary, and quaternary structure of a protein. This attribute allows researchers to characterize the structural and mechanical differences between biologic drugs and their biosimilars. The complicated higher order structure of monoclonal antibodies is determined from nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry (MS) data. Currently, there are insufficient resources that can neither measure the distances between NMR spectra nor can they cluster NMR data in a useful way. My project involves implementing a combination of mathematical and statistical techniques of data analysis to classify monoclonal antibody spectra. I will introduce and survey the efficacy of tools such as Principal Component Analysis (PCA), Tucker Decomposition, and Earth Mover's Distance (EMD).

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Eric Liu			
Academic Institution:	Carnegie Mellon University	**Major:**	Information Systems
Academic Standing (Sept. '19):	Sophomore		
Future Plans (School/Career):	Pursuing a career in Software Engineering while earning a master's degree in Informat		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Security Manageme		
NIST Research Advisor:	Dr. Ramaswamy Chandramouli		
Title of Talk:	Hardware-Based Security Measures for Virtual Machines		

Abstract:

Virtual machines (VMs) are virtual application environments that behaves like a separate computer but can be run on any host machine with a hypervisor. VMs are the most popular method of virtualizing computing resources and are the backbone of most major cloud services. As most organizations and even governments rely on cloud computing, the entire world is dependent on the security of virtual machines. Most current VM security measures are based in software, which is less secure than hardware-based security measures. Current efforts in hardware-based security measures are mostly limited to securing a single device and less commonly used.

This project proposes a hardware-based security measure for virtual machines that combines the advantages of both Trusted Platform Module (TPM) technology and Intel's Software Guard Extensions (SGX) technology. Our design uses a TPM chip located on the host machine to securely start and stop the different VMs while using SGX enclaves as a runtime environment for the VMs to ensure that they are secure throughout the VM lifecycle. Our design protects against unauthorized access of secure data inside of a VM, a malicious hypervisor, adversaries gaining access to a valid VM user's account, and even malicious code running inside of a VM.

Our design could be utilized by all virtual machines to further increase the security of the VMs and thus, the information accessed and processed by the VMs. However, our design relies on the integrity and security of SGX which means relying on Intel. Corporations might be reluctant to adopt our design as Intel controls when and how SGX enclaves are used. Future research could combine the functionalities of TPM chips and SGX enclaves into one device so that hardware security could be achieved for a cheaper price and not have to rely on a specific manufacturer such as Intel.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Lily Northcutt		
Academic Institution:	University of Maryland, College Park	**Major:**	Mathematics
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	Undecided: working after graduation or attending grad school for applied math		
NIST Laboratory, Division, and Group:	ITL, Applied & Computation Mathematics, Mathematical Analysis & Modeling		
NIST Research Advisor:	Prof. Michael Mascagni		
Title of Talk:	Modeling First Passage Brownian Motion using Walk on Spheres Method		

Abstract:

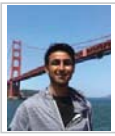
Brownian motion (BM) is a Wiener or stochastic process that can be used to solve partial differential equations (PDEs). BM pervades a multitude of disciplines and natural phenomena; most famously the random movement of particles in a fluid.

The Walk on Spheres (WOS) algorithm is a Monte Carlo method that provides a good approximate solution to PDEs with boundary conditions, and uses first passage (hitting) locations of BM to form its random estimates. WOS generates a BM's trajectory by letting BM starting at a sphere's center hit the surface uniformly. Thus, one can create a sequence of spheres until they hit the complicated boundary of the region within a specified ε.

In the half-space, the boundary is the x-y plane, and WOS reduces to a simple 1-dimensional random process in the remaining coordinate. Using this simplified process to observe the number of steps (N) in WOS, we find it fits the negative binomial distribution well. As anticipated, the mean of N is log-linearly related to ε.

The NIST ZENO code computes material properties using WOS. We use ZENO to perform WOS on various molecular structures. In these more complicated cases, the behavior of N is consistent with that of our simplified, 1-dimensional model . For the majority of molecular geometries, even those quite different from one another, the number of steps to reach the molecule also appears to be negative binomially distributed, and the mean of N produces the same ε relationship.

Considering BM close enough to a complicated boundary such that the boundary appears planar, it makes sense for the simple model to capture much of the behavior observed. We conclude that first passage locations of BM are distributed similarly to the negative binomial distribution, and that our simple set-up is a good model of first passage locations of BM.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Shyaer Parvez		
Academic Institution:	University of California, Berkeley	**Major:**	Computer Science
Academic Standing (Sept. '19):	Junior		
Future Plans (School/Career):	Plan to have career in CS/AI and potentially obtain an MBA while working.		
NIST Laboratory, Division, and Group:	ITL, Software and Systems Division		
NIST Research Advisor:	Dr. Ram Sriram		
Title of Talk:	Revamping Health Care Through Rule-Based Expert AI Systems		

Abstract:

In 2019, with Artificial Intelligence (AI) employed to increase problem solving and efficiency, a plethora of scientific fields have incorporated AI, including medicine. One element of medicine, however, that has yet to effectively utilize AI is healthcare, a field in desperate need of revamping. Prior authorization is an aspect of healthcare that is often viewed as a time-wasteful process. Prior authorization is a sort of approval procedure whereby health insurance companies determine if they will cover a prescribed medication, procedure, or other service. This involves having a physician personally assess the patient's situation and then evaluate what sort of treatment is legitimate and what kind of coverage the patient is entitled to from the insurance company. While prior authorization has its benefits, it has received criticism from doctors for being expensive and time-consuming. Using a rule-based or knowledge-based expert system (KBES), this process could potentially be streamlined to automatically validate a patient's situation and grant them prior authorization for the insurance company without the use of a doctor. MORE Integrated Development Environment (IDE) is a java-based program which is a tool for building object-oriented KBESs, supporting both forward and backward chaining systems. With its use of the efficient RETE network algorithm, MOREIDE is capable of building a KBES large enough to properly encode prior authorization. Finally, the object-oriented KBES made in MOREIDE can be integrated with natural language processing to create a patient-friendly, commercial tool which would greatly improve the allocation of a physician's time.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Sydney Pugh		
Academic Institution: Loyola University Maryland	**Major:** Mathematics & Computer Science	
Academic Standing (Sept. '19):	Graduate Student	
Future Plans (School/Career):	I will be pursuing a PhD in computer science at the University of Pennsylvania.	
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Security Components and Mechanisms Group	
NIST Research Advisor:	Richard Kuhn, M S Raunak, Raghu Kacker	
Title of Talk:	Developing Effective Test Strategies for Cryptographic Algorithm Implementations	

Abstract:

Cryptographic algorithms are essential for securing communication over any network. They are complex and dense with bit manipulations and condition predicates. Traditional test strategies such as source code path coverage are generally ineffective. Moreover, cryptographic algorithms may be classified as "non-testable" programs because it is impractical, or otherwise impossible, to generate a test oracle (i.e., a function that given a set of inputs, provides corresponding correct outputs) to verify that the algorithm's implementation functions properly. Together, these characteristics make it very difficult to effectively test and find bugs in cryptographic algorithm implementations.

Recent research has applied new testing strategies to cryptographic hash function implementations submitted to NIST's Secure Hash Algorithm-3 (SHA-3) Competition and public-key cryptographic function implementations submitted to NIST's Post-Quantum Cryptography (PQC) Standardization Process. The tests were designed from metamorphic relations that were based on the specifications of the algorithms. Several bugs were discovered in these implementations using these metamorphic tests.

In this research, we turn to NIST's Lightweight Cryptography (LWC) Standardization Process which aims to develop new public-key cryptography algorithms that are optimal for devices with constrained resources (e.g., RFID tags and IoT devices) for standardization. Specifically, the LWC Process solicited authenticated encryption with associated data (AEAD) and hash algorithms. We applied similar testing strategy to those applied to SHA-3 and PQC mentioned above. Furthermore, we developed new tests motivated by the LWC submission requirements imposed by NIST. Our test strategy offers an effective way to test cryptographic algorithm implementations and catch potential bugs before they are deployed.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Mason Rhodes		
Academic Institution: Creighton University	**Major:** Physics and Mathematics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Pursue a Ph. D. in physics, specializing in quantum computing	
NIST Laboratory, Division, and Group:	ITL, Advanced Network Technologies Division, Emerging Network Technologies	
NIST Research Advisor:	Lotfi Benmohamed	
Title of Talk:	Dynamic Cache Management with Network-Wide Capacity Constraint	

Abstract:

Allocating and managing network cache systems is an extensive area of research in developing Future Internet architectures. In an Information-Centric Network (ICN) design, and in particular with Named Data Networking (NDN), rather than requesting the physical location of data, the named content itself is requested, increasing network efficiency. The emergence of cloud-based networking, in which virtual nodes of the network are contained in cloud data center nodes and can receive updates to storage resources as necessary, creates an architecture with the potential for dynamic cache allocation and management. While prior work has used this approach to manage content placement given a cache capacity constraint at each network node, the present study assumes a network-wide cache capacity, and uses dynamic storage resource updates to determine the optimal per-node cache capacity. However, the offline version of dynamic cache allocation is NP-Hard. Instead, a distributed adaptive algorithm is developed that approximates the solution to within a constant factor of the optimal. I provide two packet level simulations of this algorithm using Python. One demonstrates the synchronous, or ideal, algorithm proven mathematically in this paper, in which it is assumed that all nodes have received a message containing the error associated with adjacent nodes before updating their state. The other demonstrates the asynchronous, or non-ideal, case that has not been proven mathematically, in which there are instances of nodes updating their state without having received a message containing an adjacent node's error. These simulations were tested over several network topologies using various free parameters to develop a comprehensive understanding of the evolution of this system and they indicate significant improvement over prior cache allocation algorithms, as expected.

SURF Student Colloquium

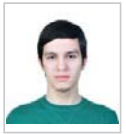
NIST – Gaithersburg, MD
August 5-9, 2019

Name: Caleb Robertson

Academic Institution: Liberty University	**Major:** Unmanned Aerial Systems
Academic Standing (Sept. '19):	Sophmore
Future Plans (School/Career):	I plan to continue developing my skills at liberty University while building a career at NIST.
NIST Laboratory, Division, and Group:	Robotic Test Facility, Computer Security Division, Security Components & Mechanisr
NIST Research Advisor:	Jeff Voas
Title of Talk:	Analysis of the Current Security Infastructure Partaining to Small Unmanned Aerial Sy

Abstract:

With the development of small Unmanned Aerial Systems around the globe, the need to declutter communication bandwidths and secure transmissions has become paramount. The methods used to study this problem are an analysis of the current sUAS infrastructure and capabilities, regulations and restrictions pertaining to usable frequency ranges, and the security of data transmission and commands to the sUAS. The results found by this study show that sUAS infrastructure for safe and secure operations is sorely lacking, that frequency clutter is a cause of sUAS accidents involving damage to property or loss of life, and that simple encryption algorithms drastically reduce the capability of unauthorized users from listening in to the communications between the ground station and the sUAS. With the airspace surrounding cities and homes is becoming more crowded each day, sUAS bandwidth restrictions should continue to be updated to meet the needs of the market. This will foster the growth of the sUAS infrastructure as the market creates a higher demand on the system. By creating sUAS infrastructure to support usable frequency expansion, the security and safety of sUAS will be in the grasp of the market within the next few decades.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Temur Saidkhodjaev

Academic Institution: University of Maryland, College Park	**Major:** Computer Science
Academic Standing (Sept. '19):	Junior
Future Plans (School/Career):	Career in Software Engineering or Computer Science Research
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division, Secure Systems and Applications Group
NIST Research Advisor:	Jeffrey Voas, Richard Kuhn
Title of Talk:	Verified Timestamping

Abstract:

Timestamping is the process of assigning time to a transaction or an event. It is commonly used to sign digital documents and has applications in blockchain and concurrent programming. The purpose of the project is to create a proof of concept implementation of a Timestamping Authority, which would aggregate time from several atomic clocks to produce a common timescale to be shared across the network or system. Since timestamping is mostly used to check the order of events, this common timescale is not guaranteed to be accurate, but rather one that preserves the order of events and one that system participants can agree on.

In order to prove the viability of the Timestamping Authority idea, the prototype software had to be created. Before that, current protocols for network time synchronization and timestamping procedures have been researched. Network Time Protocol (NTP) was chosen to be used for timestamping server-client communication, as it is used by most devices today for clock synchronization. The list of reliable and accurate atomic clocks has been found at the International Bureau of Weights and Measures. These atomic clocks participate in creation of Coordinated Universal Time (UTC) and are highly synchronized, so they can be used for timestamping purposes as sources of time.

Then, proof of concept implementation of the project in Java programming language has been created. Tests have shown that the order of events is preserved with down to ten milliseconds accuracy, which is good precision for a large network, in which this software is expected to operate.

This is the first attempt of multiple atomic clock times aggregation to produce real-time high accuracy timestamps. With more research, it can be used to aid in solving a variety of race condition situations in computing, as well as in simpler situations where reliable timestamps are needed.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Justin Slud		
Academic Institution: University of Maryland	**Major:** Math and Economics	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Pursuing a career in the tech industry.	
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division	
NIST Research Advisor:	Sanford Ressler	
Title of Talk:	Towards Integrating Virtual Reality with NIST's Digital Library of Math Functions	

Abstract:

According to their website, NIST's Digital Library of Mathematical Functions (DLMF) is an open, online resource created to be a digital version of their handbook, an "invaluable reference for the many scientists and engineers who use special functions of applied mathematics in their day-to-day work." Using a JavaScript library called A-Frame, we took the DLMF's 3D surfaces of complex equations and created interactivity within a web-based virtual reality environment which can be viewed on any browser without the need to download special software. Previous work from NIST staff and interns enabled us to visualize the models, and now users can pan around, navigate menus, and manipulate objects much like in a video game. If the user has access to a

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Cameron Smith		
Academic Institution:	**Major:** Applied Computer Science	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Software Engineer	
NIST Laboratory, Division, and Group:	ITL, Software and Systems Division, Systems Interoperability Group	
NIST Research Advisor:	John Garguilo	
Title of Talk:	Creating a software client to show conformance of healthcare info - HL7 v2 Standard	

Abstract:

Introduction:

The subject of my research/program development deals with the lack of interoperable healthcare systems. The solution to this problem lies in the exchanging of information within electronic health records validated to developed standards. The core mission of my group, the software interoperability group, is to advance test methods, systems, and software, making tools to help show conformance to standards. The Ultimate goal is interoperability. People should be able to access and communicate health data in a common way using electronic health records, at any place and time. This summer, I developed a new C# Sample Client which enables users to validate messages via the NIST tools demonstrating conformance to standards.

Methods:
• Create a Client with C# in Visual Studio using a WSDL
• Access NIST Conformance Methods (Specifically Validation)
• Develop efficient code "Structure" for the Client
• Identify errors within in the developed C# program and display to user

Result/Goal:
To develop and code a NIST C# Web Service Client Program that can validate HL7 v2 Messages input by the user. This C# client has the capability for a user to open a file dialog and input their files required for the NIST validateWithResources() method. The created client parses the user input profile to obtain the "MessageID" to use for the method. The program returns a report to the user which they can save to

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Peter Stein			
Academic Institution:	University of Maryland, Baltimore County	**Major:**	Computer Science
Academic Standing (Sept. '19):	Sophomore		
Future Plans (School/Career):	Pursuing a career in the tech industry after earning a master's in computer science.		
NIST Laboratory, Division, and Group:	ITL, ACMD, High Performance Computing and Visualization Group		
NIST Research Advisor:	Steven Satterfield		
Title of Talk:	Developing a Common CAVE and Web-Based Virtual Reality Menu System		

Abstract:

The Cave Automatic Virtual Environment (CAVE) is a room designed to view objects and data in virtual reality. At NIST, it consists of two walls and a floor that have images projected upon them to appear three dimensional to a viewer wearing tracked glasses. When wearing the glasses, a researcher can walk among the data and gain different perspectives, which can help them better understand their data. Unfortunately, the CAVE is built into a room, so researchers have to visit the room to use it. One way to make virtual reality more available is web-based virtual reality (web VR), where a browser can host a program that can run on a desktop, a phone, or a virtual reality headset. The latter two can be used to give the viewer similar perspectives to the CAVE, but can be used from any location with access to the webpage.

Many tools have already been developed for the CAVE, which make it easier to build complex, interactive visualizations quickly. These visualizations are not compatible with web VR, so another development cycle is required for the data to be viewed across the web. This could be avoided if the commands used to build the CAVE visualization could also be used to build a web VR program as well. The focus of this project was to develop a working prototype program that when fed commands, builds both a CAVE-based program and a web VR-based program, using the most common features from the CAVE. This prototype program can significantly cut down on development time for new visualizations, while increasing their availability by allowing them to run through web browsers.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Henok Tasissa			
Academic Institution:	University of the District of Columbia	**Major:**	Computer Science
Academic Standing (Sept. '19):	Junior		
Future Plans (School/Career):	I plan to attend graduate school and work in big technology companies.		
NIST Laboratory, Division, and Group:	ITL, Software and Systems Division, Information System Group		
NIST Research Advisor:	Timothy.Blattner		
Title of Talk:	Hedgehog Generator: Tool used to generate boilerplate code.		

Abstract:

Hedgehog is an approach that aims at obtaining performance on systems with multiple CPUs and GPUs. The Hedgehog framework provides the functionality to build the task graph, which is made up of a series of vertices and edges. A vertex represents a task (or a graph), which can manage a state or execute computation on data that is sent to the task. Edges connect these tasks to encode data dependencies. The Hedgehog API implements this framework.

Hedgehog requires writing lots of boilerplate code which is associated with the Hedgehog API. The boilerplate code represents creating tasks, state, state managers, the main function that builds the graph, and a CMakeList.txt file to compile the project. Writing this code is time consuming, repetitive, and grows in complexity as the graph gets larger.

To help developers/researchers avoid the time consuming, repetitive, and complex task of writing a lot of boilerplate, we have developed a web-based graphical user interface (GUI) application which takes care of generating the boilerplate code. This application allows developers to create new tasks, define input and output types, create states and state managers, select task interface functions, and draw edges between tasks. The developer can then Export the graph, which will generate the necessary code to compile and run the graph. These generated files are compressed as a zip file which can be downloaded easily.

The Hedgehog Generator is a fast and intuitive tool which helps developers to focus more on implementing the tasks, rather than concerning themselves with writing boiler-plate code. It reduces the amount of work needed to write the boilerplate code and helps visualize the structure of their project without implementing its functionality. The tool also provides validation checks that ensures a graph is valid for their projects.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Daniel Tokarz	
Academic Institution: Yale University	**Major:** Applied Math/Mech Engineering
Academic Standing (Sept. '19):	Senior
Future Plans (School/Career):	I plan to pursue a career as a data scientist in the private sector.
NIST Laboratory, Division, and Group:	ITL, Computer Security Division, Security Engineering & Risk Management Group
NIST Research Advisor:	Hung Trinh
Title of Talk:	Developing a Graph Database to Evaluate/Analyze Cyber Incidents

Abstract:

The availably of information relevant to Cybersecurity Risk Analytics does not match its growing importance in the private and public sectors. To combat this, our team at NIST is working to establish standardized methods and tools to analyze patterns and trends in cyber incidents.

Our team's work includes creating a central database that pulls information from a variety of sources. Organizations such as the Identity Theft Resource Center, the Web Hacking Incident Database, and the Department of Health and Human Services collect their own data with unique fields. While the information may be different, ~10% of the incidents described in a given database are also reported in another database. The main goal of the project is to develop methods to centralize these sources into a single database, taking advantage of the unique information included in each source. Because each database has thousands of entries, it is important to develop methods that perform much of the cleaning and merging automatically. This includes using Natural Language Processing to detect common entries in different databases and fitting a logistic regression model that analyzes the similarities between database entries.

After using RStudio to clean our respective databases, we have selected Neo4j as the system on which to create our master database. The Neo4j system hosts graph databases, which are principally comprised of nodes and their relationships, rather than entries with values from different fields. This allows us to visualize the similarities between incidents in a way that grants direct insight into patterns. While the product of this project is not a completed database, we have developed a proof of concept so that similar methods used by future researchers can contribute a chapter to the conversation that will prove valuable in effectively evaluating cyber risk. This proof of concept is organized in a shared GitLab environment.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Richard Williams Jr.	
Academic Institution: University of Maryland, College Park	**Major:** Computer Engineering; Music
Academic Standing (Sept. '19):	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:	The Effect of Different Bias Estimation Methods on Linear Cryptanalysis

Abstract:

Cryptography has become increasingly important to all aspects of computer security. Cryptographic systems are only secure when they can protect secret information from attackers; therefore, cryptographers must understand potential attacks via cryptanalysis. Linear cryptanalysis is an attack that can be used on block ciphers, which encrypt one block of plaintext data at a time using a secret key. Linear cryptanalysis aims to approximate the operation of a block cipher using linear equations, where each equation holds with a certain probability. If an attacker can analyze enough encrypted data to detect these probabilities, then they can discover information about the secret key—weakening or potentially destroying the security of the data.

For most block ciphers, security comes from performing many rounds of encryption. Simeck is a block cipher for which a full linear cryptanalysis is not feasible, but there exists a linear attack if the number of rounds is reduced. The purpose of this research was to investigate how different distributions of plaintext data change the effectiveness of linear cryptanalysis attacks on reduced-round Simeck. Using bias estimation techniques such as the Hansen-Hurwitz estimator and stratified sampling, I searched for plaintext patterns that would strengthen or weaken linear attacks. This knowledge is crucial because real-world data will often follow some pattern or distribution, whether it is numerical, textual, etc. Thus, the designers of cryptographic systems must be aware of situations that may compromise security.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Jesse Zhu		
Academic Institution: Cornell University	**Major:** Computer Science	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Software Engineer	
NIST Laboratory, Division, and Group:	ITL, Software and Systems Division, Cyber Infrastructure Group	
NIST Research Advisor:	Dr. Ram Sriram; Dr. Eswaran Subrahmanian; Dr. Talapady Bhat; Mr. Jacob Collard	
Title of Talk:	User interface development for Root and rule (R&R) based system for curating, indexing and searching documents	

Abstract:

R&R (root and rule) is a domain-independent terminology generation method in which meaningful phrases are extracted and standardized into terms through linguistic techniques for a specific domain. Parmenides is the library that executes the R&R extraction, and there are over twenty settings that can be changed when running the software. In addition to inputting a large number of files, if a user wishes to change a large amount of the default settings, the process can become convoluted. As such, the development of a user interface for running Parmenides is vital for the extensibility of the program to all users. The goal of this project is to develop such an interface that is as intuitive as possible, while maintaining the flexibility of modification as new changes in the Parmenides software develop. A flow diagram was generated with each setting input and interaction being carefully considered, and the code was designed in a modular fashion to be easily readable and extendable, with a feature such that the user could control what is displayed on the actual interface through CSV files. After the implementation of the user interface, rigorous testing was conducted to make sure that the interface was functionally correct, and modifications were made accordingly.

Further reading: DOI: 10.1007/s11837-015-1487-4; Journal of Washington Academy of Science,. Vol 104, Number 4, Winter 2018 – pp 31 to 78.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Kevin Zong		
Academic Institution: University of Maryland, College Park	**Major:** Computer Engineering	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Finishing undergraduate studies and pursuing a career in software engineering	
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, Computing an	
NIST Research Advisor:	Oliver Slattery, Abdella Battou, Lijun Ma	
Title of Talk:	Network Management System Towards the Platform for Quantum Network Innovation	

Abstract:

Ongoing developments in connected and distributed quantum technologies and in dynamic transmission of quantum signals are paving the way for generalized quantum networks. Therefore, there inherently comes a need to test the new and existing quantum devices and protocols that operate within these quantum networks. This is the goal of the Platform for Quantum Network Innovation (PQNI), which will be a quantum extension of the existing Platform for Network Innovation (PNI) on the NIST campus. Among the first steps in implementing the PQNI is the development of a network manager. The initial objective of this network manager is to monitor and control the functionality of the PNI in a scalable manner and in such a way as to also be compatible with the all-optical systems required for the PQNI.

The network manager consists of three Vert.x microservices: one utilizes a Simple Network Management Protocol (SNMP)-based algorithm to discover the complete layer 2 topology of the network, another provides a web-based graphical user interface (GUI) to view the topology and interact with individual network nodes, and the third maintains a database for the manager. Together, these microservices form a cohesive web application that allows users to view a live visual of the entire network topology, test the performance of components and protocols in the network, and configure each individual component.

With this real-time network management system, managing the many components and protocols in the PNI is now more convenient and efficient with the system's easy-to-use interface. Looking towards the future, as development of the PQNI advances, we will apply this network management system to actively manage the PQNI.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Kevin Zong		
Academic Institution: University of Maryland		**Major:** Computer Engineering
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Obtaining a Post-Graduate Degree	
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division,	
NIST Research Advisor:	Gavin O'Brien & Michael Nieles	
Title of Talk:	NVD, CPEs, and CVEs: Maintaining a Searchable Vulnerability Database	

Abstract:

As Internet connectivity becomes increasingly prevalent in everyday applications and devices, the threat of an individual or entity being exploited by a vulnerability in the code of the applications or devices by a malicious actor increases. A vulnerability is defined as "a weakness in the computational logic (e.g., code) found in software and hardware components that, when exploited, results in a negative impact to confidentiality, integrity, or availability." The National Vulnerability Database (NVD) is a publicly available database created to allow any entity to check whether the devices and applications which they rely on contain vulnerabilities. The NVD performs analysis on vulnerabilities that have been published using publicly available data and lists them in a searchable database where each vulnerability is labeled with unique identifiers. Each vulnerability is assigned a specific Common Vulnerabilities and Exposures (CVE) ID number which helps the public specify and keep track of specific vulnerabilities in any context and each CVE entry contains an applicability statement or Common Platform Enumeration (CPE) which specifies what product(s) the vulnerability effects. This combination of CVEs, IDs, and CPEs, allow any entity to search for the products and services they rely on and ascertain whether they contain any vulnerabilities which need to be patched. Maintaining this database and ensuring the uniqueness and accuracy of the identifiers is critical to the NVD and keeping the cyber infrastructure secure. Complicating this effort is the ever-changing landscape of software, hardware and their interactions along with a constant stream of new vulnerabilities. As these changes occur the NVD and corresponding existing CVEs and CPEs must be updated while new CVEs and CPEs must be created. My project will explain to everyday people the importance of this work and the uses of the NVD in making sure that the hardware and software they use are vulnerability free.

MML- NCNR

MML SURF Participants	
First Name	Last Name
Nina	Agrawal
Thomas	Bina
Huilang	Chen
Julia	Colon-Martinez
Julia	Danischewski
Nicholas	D'Antona
Caitlin	Darling
Ava	Farahbakhsh Darabi
Eli	Fastow
Ethan	Finlay
Nathan	Gill
Darnell	Harris
Jacob	Hechter
Chad	Hite
Allison	Horenberg
Klara	Keim
Eleanor	Kelman
Jinsung	Lee
Siminben	Manasiya
Joelle	Marchiani
Oriana	Ovide
Rajashow	Parajuli
Samuel	Philliber
Joshua	Price
Adam	Robinson
Katrina	Rupert
Usmaan	Siddiqui
Ryan	Smith
Noah	Smith
Lu	Song
Jonah	Tash
Winnie	Tran
Nidhi	Vantair
Yuke	Wang
Gamitha	Wijekoon
Fjorela	Xhyliu
Julie	Yagodich

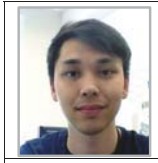
SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Nina Agrawal		
Academic Institution: University of Maryland College Park	**Major:** Computer Engineering	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Graduate school or workforce	
NIST Laboratory, Division, and Group:	Material Measurement Lab, Computational Materials Science	
NIST Research Advisor:	Jack Douglas	
Title of Talk:	Characterizing the Cooperative Motion in Condensed Fluids using Machine Learning	

Abstract:

Within the scientific community, it has been widely debated as to why the relaxation time or viscosity increases as glass forming polymers are cooled. However, it has been observed that as the material is cooled, it exhibits dynamic heterogeneity. When a material is dynamically heterogeneous, particles within the polymer have a wide distribution of mobility. Research has shown that the particles with low mobilities tend to cluster together while particles with high mobility exhibit similar behavior. Within the particle clusters of the highest mobility, a subset of these particles exhibit cooperative motion. The string model for cooperative motion established a quantitative relationship between the size of the cooperatively rearranging particle chains and the relaxation time. Our research involves using machine learning algorithms such as DBSCAN to quantify the size of the cooperatively rearranging particle chains of Poly Methyl Methacrylate (PMMA) We hope that this will enable us to better understand why the relaxation time increases as PMMA is cooled.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Thomas Bina	
Academic Institution:	Pennsylvania State University	**Major:** Materials Science & Engineering
Academic Standing (Sept. '19):	Senior	
Future Plans:	Graduate School	
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science and Engineering Division	
NIST Research Advisor:	June Lau & Gretchen Greene	
Title of Talk:	Development of the Microscopy Laboratory Information Management System	

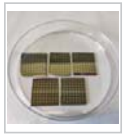
Abstract:

The NIST Electron Microscopy Nexus coordinates a suite of 10 microscopes that facilitate materials science research. Currently, the significant amount of data generated by this facility often reaches a dead end on local storage due to the absence of a proper system designed to manage this data, which effectively becomes irrecoverable over time. To improve upon and replace this system, we are developing a data management system designed to effectively manage the data generated by the Electron Microscopy Nexus, enabling data-driven materials research and discovery in the long-term.

For a given microscopy session, there is a wealth of data generated beyond captured images; session notes, sample information, subsequent analysis, etc. contribute to a holistic understanding of an experiment. However, manually collecting relevant data is difficult and time-consuming. Fortunately, this information may be digitally accessed. Thus, we can programmatically mine this data to build a complete record of a microscopy session in such a way that follows FAIR data principles: findable, accessible, interoperable, and reproducible. (1) This includes bringing metadata generated by the microscope itself together with information from outside sources including electronic lab notebooks and online scheduling calendars.

To develop this repository of electron microscopy data, relevant data itself is captured and parsed from each distinct source to be fit into a well-developed XML schema. Via this schema, we populate XML files with the captured information. Using the NIST Configurable Data Curation System (2) as the base platform, we created and host a web directory of the pertinent data and metadata from each microscopy session, allowing for ease of both search and display. In doing so, electron microscopy data and metadata become more accessible, and thereby we enable more effective material discovery. This system's eventual deployment has farther reaching applications; we hope that machine learning applications will take advantage of the ease of access afforded by this system for further data-driven materials discovery.

1. Wilkinson, Mark D., et al. "The FAIR Guiding Principles for Scientific Data Management and Stewardship." Scientific Data, vol. 3, no. 1, 2016, doi:10.1038/sdata.2016.18.
2. CDCS, NIST Information Technology Lab, mdcs.nist.gov/.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Huilang Chen

Academic Institution:	University of Maryland, College Park	**Major:**	Computer Engineering
Academic Standing (Sept. '19):	Junior		
Future Plans (School/Career):	University of Maryland, College Park		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory Materials Science and Engineering division Polyme		
NIST Research Advisor:	Lee Richter, Ahmad Kirmani		
Title of Talk:	Blade-coated In2O3/ZnO bilayer heterostructures		

Abstract:

Metal-oxide semiconductors have been actively explored for low-cost transparent flexible electronics owing to their excellent charge transport compared to amorphous Si. The amorphous ternary alloy: InGaZnO has received considerable commercial interest but requires plasma deposition and high temperature annealing. This has led to research in low-temperature solution- processing. The simpler binary compound Indium oxide (In2O3) represents an interesting test case as it can be thermally processed to form either amorphous (a) or nano-crystalline (x) films, allowing one to explore the role of structure in device performance. In this study, we explore scalable fabrication of In2O3 thin-film transistors (TFTs) using a sol-gel synthesis route and blade coating. Optimization of film thickness leads to improved threshold voltages and electron mobilities, μ, of ~3 cm2V-1s-1 in enhancement mode for both (a) and (x) films. Commercial applications demand mobilities > 10 cm2V-1s-1. It has been reported that In2O3/ZnO bilayer structures can lead to improved mobilities, attributed to the formation of a confined 2D electron gas. We are exploring blade-coated In2O3/ZnO bilayer heterostructures, in order to determine the role of the underlying In2O3 structure in the bilayer performance. We find that the nanocrystalline nature of the In2O3 layer, achieved at higher annealing temperatures (300°C), is crucial to achieving high μ~15 cm2V-1s-1. Devices made following the established optimized coating conditions will enable detailed electrical measurements to probe the role of electron confinement in the improved performance.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Julie Colón Martínez

Academic Institution:	University of Puerto Rico - Mayagüez	**Major:**	Chemical Engineering
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	Pursue graduate studies in Nanotechnology.		
NIST Laboratory, Division, and Group:	Material Measurements Lab, Chemical Sciences Division, Chemical Sciences Division HQ Group		
NIST Research Advisor:	Huong Giang Nguyen		
Title of Talk:	Selectivity Prediction on Binary Gas Adsorption of CO2/N2 on Zeolite Reference Materials		

Abstract:

Our world is currently facing environmental challenges, such as climate change and air pollution, due to excessive emissions of gases like CO2 and NOx. This urges the exploration of better energy sources that do not involve fossil fuels. Adsorption, especially physical adsorption, is seen as a cleaner and less energy-consuming separation mechanism to solve our alternative sources of energy crisis, or as an emissions mitigation tool in our fossil fuels industry since some of the alternative energy sources currently investigated are not developed enough to meet our energy demand. In this present work, the selectivity of CO2 and N2 at high pressure is being predicted on NIST zeolite reference materials RM 8852 (Ammonium ZMS-5) and RM 8850 (Zeolite Y) in order to obtain binary adsorption isotherms at 25 °C and 35 °C. This is done by evaluating the high-pressure pure adsorption equilibria of CO2 and N2 on a gravimetric instrument and a manometric instrument with both mentioned zeolites. Data obtained from the different adsorption equipment will be compared to ensure the accuracy of the data. Binary CO2-N2 adsorption equilibria will be predicted using the ideal adsorbed solution theory. The pore structures of the reference materials and intermolecular forces between the gases and the materials are going to be analyzed to better understand the selectivity results. It is expected for CO2 to be the more adsorbed gas in the mixture due to its interaction with the material's surface, mostly for RM 8850.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Julia Danischewski		
Academic Institution: Skidmore College	**Major:** Chemistry, German	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Attend graduate school and pursue a Ph.D.	
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Material Science and Engineering Division, Polyr	
NIST Research Advisor:	Nicholas Posey	
Title of Talk:	Finding the Binding: Synthesis and Dynamic Light Scattering Analysis of Polyelectrol	

Abstract:

No longer just for water bottles and plastic bags, polymers are serving a growing role in the field of biomedicine. Aliphatic polycarbonates (APCs) especially have gained traction in this field due to their biodegradability and rich potential for functionalization. Highly-charged, polyelectrolyte APCs are used for drug delivery and in injectable hydrogels but have undergone limited charge optimization with respect to their ability to bind and deliver proteins. In this study, charged amino-acid inspired side chains were conjugated to APCs, bearing pendant alkene groups, via radical-mediated thiol-ene chemistry, to achieve high degrees of functionalization and increase APC tunability. The resulting polyelectrolytes were characterized through dynamic light scattering (DLS) to measure their hydrodynamic radius (DH) in biologically relevant solutions. The highly cationic polymer formed complexes with bovine serum albumin as shown by DLS. Future work will focus on building a family of polyampholyte APCs with mixed, charged sidechains for enhanced protein binding. These new sidechain formulations will be used in triblock copolymer architectures with self-assembling properties. Ultimately, these highly tuned polyelectrolytes will offer a novel strategy for binding and delivering monoclonal antibodies for biomedical applications, helping to guide the rational design of future biomedical polymers.

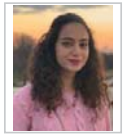
SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Nick D'Antona		
Academic Institution: St. Mary's College of Maryland	**Major:** Chemistry and Physics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	PhD in chemistry and hopefully research in renewable energy storage	
NIST Laboratory, Division, and Group:	MML, MSED, Polymers Processing group	
NIST Research Advisor:	Lee Richter	
Title of Talk:	Analysis of electrochemically doped polymer thin films via in situ ellipsometry	

Abstract:

Organic electrochemical transistors (OECTs) are an attractive new technology due to their potential for use in integrated biosensors, printed logic circuitry, and flexible electronic devices. OECTs operate by modulating the conductivity of an organic semiconducting active layer via ion injection from an aqueous electrolyte gate, unlike conventional field effect transistors (FETs) where mobile charges are induced by a gate capacitance. OECT operation involves swelling of the polymer film due to the injection of bulk counter-ions and their corresponding hydration spheres. Thus, there is growing interest in chemically tailoring the side chains of established semiconducting polymers to control and optimize OECT performance. Poly-3-hexylthiophene (P3HT) is an established FET material that performs poorly as an OECT due to its hydrophobic hexyl side-chains. We explore two synthetic variants, P3MEEMT and P3HHT, where hydrophilicity is introduced via ethylene glycol (P3MEEMT) or hydroxyl (P3HHT) moieties. We explore the utility of spectroscopic ellipsometry (SE) to characterize the electrochemical doping and swelling of the polymers. In principle, SE can determine both the degree of oxidation from changes in the polymer dielectric function (ε) and swelling from changes in film thickness. In practice, correlations between ε and thickness can confound the measurement. We are exploring data acquisition and reduction approaches combining SE and electrochemistry (EC) to allow a complete characterization of the materials. Using SE and EC we can compare the effect of different electrolytes on film swelling. Namely we compare KCl to KPF6, a kosmotropic ion with large hydration sphere and chaotropic ion with a small hydration sphere, respectively. We investigate this swelling effect in films processed to varying degrees of polymer order.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Ava Farahbakhsh Darabi		
Academic Institution: Montgomery College	**Major:** Biology	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	University of Maryland School of Dentistry	
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Material Science and Engineering Devision, Polym	
NIST Research Advisor:	Thomas Moffat, Nicole Ritzert	
Title of Talk:	Developing Oral Sensors Based on Glucose and pH Levels	

Abstract:

Dental caries, periodontal disease, and diabetes are example of diseases that can cause serious problems for the patient if diagnosed late. To diagnose these diseases in time, our overall goal is to develop oral sensors to detect diabetes and oral caries based on glucose and pH. Since diagnosis can vary from dentist to dentist, we want to make more quantitative and reproducible measurements. Our approach is using electrochemical sensors. The work is done by modifying electrode surfaces with enzymes and protective layers and then testing them in physiological media. Meanwhile, we want to be certain that the sensors are reproducible and stable under different conditions. The focus of my project started with glucose sensors. The idea is that glucose produces hydrogen peroxide (H2O2) by reacting with glucose oxidase (GOX). The H2O2 oxidizes and produces a current that we measure. The GOX layer is composed of different components. In order to optimize the concentrations, multiple tests were run with different concentrations of GOX. The current is related to the amount of glucose, so the electrodes were tested in different concentrations of glucose to generate a calibration curve. Next, we tested o-phenylenediamine (OPD) layer because we found that molecules such as ascorbate interfered with current. By depositing the OPD the signal with ascorbate decreased and H2O2 stayed the same. The last layer tested is the Perfluorosulfonic acid membrane such as Nafion. We drop casted Nafion on the electrodes with OPD and GOX layer on. After testing the current in glucose, the current decreased after adding two layers of Nafion but did not drop with adding one layer. Therefore, we want to know if thickness affects the current by checking the current in potassium ferricyanide solution. There was a significant drop after depositing the first layer unlike the bare GOX. In addition to testing the concentration of the Nafion film, parameters such as the effect of pH on the signal are being tested.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Caitlin Darling		
Academic Institution: Clemson University	**Major:** Biological Sciences	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Continue studies in graduate school	
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biomolecular Measurement Division, Biomolecular Structure and Function Group	
NIST Research Advisor:	Ella Mihailescu	
Title of Talk:	The role of Copper and Nickel in lipid oxidation relevant for antimicrobial action	

Abstract:

As essential trace elements, copper (Cu(II)) and nickel (Ni(II)) are necessary to the well-being of all living organisms. Because the body only requires minimal amounts of these elements, their intracellular transport is tightly regulated. Excess concentrations of these metals have been shown to negatively impact cellular health through several mechanisms, including lipid peroxidation. Copper and nickel are very active oxidizing agents resulting in the oxidation of the phospholipid cellular membrane when exposed to higher concentrations of the transitional metals. These oxidation events lead to the dissolution of membrane integrity and increased cellular mortality. This effect is amplified when copper and nickel ions bind to specific antimicrobial peptides with amino-terminal Cu(II)- and Ni(II)-binding (ATCUN) motifs. The destruction of cellular membranes by free copper and nickel ions as well as ions bound to peptides give these trace metals antimicrobial properties that are not yet well understood.

In this project, we analyzed the structural changes in phospholipid bilayers in response to exposure to copper and nickel in varying concentrations. In addition to the presence and amount of copper or nickel, we also used several different types of phospholipids which varied in charge and degree of saturation. Using X-ray diffraction, we investigated any structural disturbances indicated by peak splitting and phase shifting. We employed neutron reflectometry to determine similar characteristics. Additionally, we used spectrophotometry and mass spectrometry to measure occurrence and rates of oxidation. Finally, we used microscopy to measure the cytotoxic effects of copper and nickel ions as well as antimicrobial peptides that can bind these ions in live eukaryotic cells.

SURF Student Colloquium

NIST – Gaithersburg, MD August
5-9, 2019

Name: Eli Fastow

Academic Institution: The University of Maryland College Park

Major: Material Science and Engineering

Academic Standing (Sept. '19): Senior (fourth year)

Future Plans (School/Career): Doctorate in material science

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

NIST Research Advisor: Dr. Vladimir Oleshko and Professor John Cumings (University of Maryland and NIST)

Title of Talk:
Cross-comparison and Validation of Complementary Analytical Methods to Detect Lithium

Abstract: The lightest metal, lithium (Li) constitutes a key elemental component in a number of emerging technologies, including batteries, medicine, and enhanced engineering alloys. Accurately characterizing Li is therefore of great importance. However, until recently, energy dispersive X-ray (EDX) spectrometers did not have the sensitivity required to detect the low intensity signal produced by the Li K X-ray photons. The advent of high counting rate high speed windowless silicon drift (SDD) EDX detectors within the past decade allowed for the detection of Li, though it remains a significant challenge. In this study we compare several analytical techniques for the detection of Li to improve interpretation of results and identify the Li detection limits. We used windowless SDD EDX in a dual beam scanning electron microscope (SEM)/focused ion beam (FIB) and a scanning transmission electron microscope (STEM)-electron energy loss spectrometer (EELS) to measure Li in a reference material, aluminum 20 wt% lithium (AlLi) alloy powder. The AlLi alloy was prepared for analysis of its microstructure, morphology, and composition in a glove box and transferred to the STEM in a hermetic sample holder to prevent oxidation. High resolution TEM (HRTEM), selected area electron diffraction (SAED), and STEM/EELS spectroscopic imaging (SI) confirmed the dominant β-AlLi phase (NaTl-type, space group Fd3m) and the relative uniformity of Li distributions in the alloy. SAED and STEM/EELS-SI indicated a phase separation in the alloy, with the formation of lithium and aluminum oxide and low-Li content Al-Li intermetallic phases. Analysis of Li in the alloy with EELS and corresponding simulated spectra allowed us to quantify the Al:Li ratios. We analyzed the AlLi alloy with a windowless SDD EDX and corresponding simulations to qualitatively detect Li. We experimentally estimated the concentration detection limit of Li in AlLi via windowless SDD EDX on the order of .1 at% and via EELS on the order of .01 at%.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Ethan Finlay

Academic Institution: Appalachian State University

Major: Physics and Chemistry

Academic Standing (Sept. '19): Ph.D. Student

Future Plans (School/Career): Obtain a Ph.D. in Organic Chemistry at Colorado State University

NIST Laboratory, Division, and Group: Materials Measurement Laboratory, Materials Science and Engineering Division, Poly

NIST Research Advisor: Jirun Sun, Xiaohong Wang

Title of Talk: Approaches to Minimize Polymerization Stress in Dental Resin Composites

Abstract:

Polymerization stress of methacrylate dental resin composites is a major concern for dental restorations due to its catastrophic effects that may lead to tooth fracture and microleakage which is one of the major causes for secondary caries. The objective is to reduce polymerization stress through: 1) introducing a co-initiator, 2) applying composition-controlled photo-polymerization, and 3) increasing the filler contents. I will use the traditional methacrylate dental resin mixture of bisphenol A-glycidyl methacrylate (Bis-GMA) with triethylene glycol dimethacrylate (TEGDMA), 7:3 ratio by mass, as a control, with the initiator camphorquinone/amine (CQ/amine) used to enable visible light photo-polymerization. The stress reduction capability of co-initiator, pH-sensitive quaternary pyridinium salt (QPS), is evaluated. This capability is compared with the stress reduction achieved by composition-controlled copolymerization using of resin mixture of equimolar urethane dimethacrylate (UDMA) and triethyleneglycol divinylbenzyl ether (TEG-DVBE), through varying the light intensity and irradiation time. In addition, the effects of stress reduction by increasing filler contents, from 65 wt% to 75 wt%, is discussed. A self-calibrated VRC and NIST-developed setup with a tensometer and near infrared spectrometer was used to simultaneously evaluate the polymerization stress and degree of vinyl conversion of the dental resin composites. The combined effects of filler, monomer, and initiator composition were assessed. Experimental results showed that QPS reduced polymerization stress by approximately 55% ± 3% in comparison to the Bis-GMA/TEGDMA control through delay photopolymerization. In addition, the composition-controlled photo polymerization also reduced the polymerization stress. I will discuss the efficacy of stress reduction induced by these two approaches in responding to the light intensity changes or filler content changes. The optimization of dental composite composition and production will be also discussed. In summary, these results suggest that the co-initiator and composition-controlled photopolymerization showed significant improvements in reducing

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: : Nathan Gill

Academic Institution: Gordon College | **Major:** : Biochemistry

Academic Standing (Sept. '19): Senior

Future Plans (School/Career): Graduate School

NIST Laboratory, Division, and Group: MML Biomolecular Measurement Division

NIST Research Advisor: Dr. Jennifer Tullman and Dr. Christina Bergonzo

Title of Talk: Understanding ClpS N-Terminal specificity through combined simulation and experiment

Abstract:

ClpS, a small (13 kDa) protein found in bacteria degradation pathways, recognizes specific N-terminal amino acids and delivers the recognized peptide to a protease complex. Due to its binding specificity based on amino acid type *and* location in the ligand, ClpS represents a novel reagent for protein identification that is currently being pursued by NIST for its use in proteome sequencing. Using molecular dynamics (MD) simulations combined with experimental research, we sought to better understand the association of N-terminal tyrosine residues to the binding pocket of ClpS mutants. To do this we used MD software to simulate the molecular movements and interactions of protein-ligand residues over the course of a micro second. Complementing this computational examination we produced and isolated ClpS mutant proteins in the lab, and measured their binding to N-terminal residues. From this computational and empirical data, we were able to better understand what factors contribute to the ClpS tyrosine binding and theorize about methods to further enhance specificity. If these methods are successful in increasing ClpS specificity for tyrosine, it may be used as a relatively fast and inexpensive reagent for high throughput protein sequencing.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Darnell Harris

Academic Institution: Ithaca College | **Major:** Biochemistry

Academic Standing (Sept. '19): Graduated

Future Plans (School/Career): Univerisity of Maryland Biochemistry Graduate Program

NIST Laboratory, Division, and Group:

NIST Research Advisor: Thomas Cleveland

Title of Talk: Design and Production of Viral Scaffolds for Cryo-EM

Abstract:

Cryo-EM is a powerful tool for determining the structures of large macromolecules such as proteins or protein complexes. The main advantage of cryo-EM is that it does not require the sample to be in an ordered arrangement for structural determination, which is ideal for particles that are difficult to crystalize, for example. This is done by aligning and averaging individual particles computationally to achieve the necessary contrast and resolution. However, this process is usually limited to large particles (>100 kDa) since images of small particles do not contain enough information for computational alignment. This project aims to investigate a way to increase small molecule imaging resolution by designing a large viral scaffold that can bind to a small molecule in a specific way. This binding would then provide reliable data about the molecule's structure in reference to the viral scaffold. A truncated version of the Hepatitis E Virus ORF2 protein, "p239," can be produced and refolded in vitro to form virus-like particles that will serve the purpose of the scaffold. This scaffold will be engineered to include an immunoglobulin-binding Protein G domain to bind the Fc region of an IgG antibody. This IgG antibody will represent a small particle in this model, and the binding of this particle to the viral scaffold may yield improved imaging resolution via cryo-EM. I will present results of the initial Protein G engineering process and preliminary imaging of the scaffold molecules.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Jacob Hechter

Academic Institution:	Northwestern University	**Major:**	Materials Science and Engineering
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	I plan to obtain a Masters and pursue a career in computational materials science		
NIST Laboratory, Division, and Group:	Materials Science and Engineering Division, Thermodynamics and Kinetics Group		
NIST Research Advisor:	Lucas Hale		
Title of Talk:	Interatomic Potentials for Calculating Diffusion Behavior		

Abstract:

The diffusion of atoms in a crystal structure is primarily reliant on the formation and migration of point defects, such as vacancies. The experimental determinations of diffusion coefficients are often both difficult and expensive. Molecular Dynamics (MD) simulations can be used to obtain predictions of atomic-level diffusion mechanisms and directly estimate the formation and migration energies of point defects. However, the results of MD simulations depend on the interatomic potentials which are used to define the energy of the system. NIST's Interatomic Potentials Repository (IPR) project currently includes a large collection of different interatomic potentials, and a python-based framework to run several types of high throughput property calculations. Here, new and improved calculations have been developed for the framework to compute the stress field around a point defect, and its mobility energy. Using the high throughput tools, predictions are compared across different interatomic potentials and simulation sizes. The computed values are also compared to more complex simulations and available reference values to investigate the accuracy of the interatomic potentials and theoretical models.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Chad Hite

Academic Institution:	West Virginia University	**Major:**	Mechanical/Aerospace Engineering
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	I plan to pursue a PhD in a field related to material science.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Funct		
NIST Research Advisor:	Dr. Marcos Reyes-Martinez		
Title of Talk:	Elucidating the Role of Hinge Mechanics on Impact Mitigation		

Abstract:

Recent work has revealed that computational bond removal from disordered networks of nodes connected by bonds results in metamaterials with highly-tailored mechanical properties. This high degree of tunability of global mechanical properties such as Poisson's ratio is key in creating materials for impact mitigation. However, the local contributions to these properties by the hinge-like elements comprising the networks are not well understood. In this work, we utilize a computer-aided drafting program and 3D printing to produce simplified representations of hinge elements and study the relationship between geometric constraints, dynamic energy dissipation, and stress wave propagation. We perform drop-tower experiments combined with high-speed imaging to relate the deformation of hinges to the mechanical behavior under dynamic loading conditions and compare it with its quasi-static compression behavior. Our study found that rotation-dominated hinge-elements reduce the transmittance of the stress wave more efficiently than bending-dominated elements. In addition, we are able to identify the relative contributions of each deformation mode to energy dissipation. This allows us to develop an understanding of how energy dissipation depends on geometry and to generate physical models of mechanical metamaterials tailored to specific impact mitigation applications. Finally, we quantify the relative contributions of the bending and rotational stiffness of each of the different elements in defining the global energy dissipation and stress wave transfer capacities of the metamaterial over nearly four decades change in strain rates.

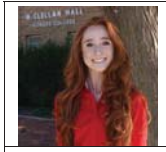
SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Allison Horenberg		
Academic Institution: University of Virginia	**Major:** Biomedical Engineering	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Attending graduate school resulting in a PhD in Biomedical Engineering	
NIST Laboratory, Division, and Group:	MML, Biosystems and Biomaterials Division, Biomaterials Group	
NIST Research Advisor:	Carl Simon	
Title of Talk:	Measuring Cell Viability in Collagen Scaffolds	

Abstract:

The inability to reliably measure cell viability in engineered tissues remains a major roadblock to the regenerative medicine and tissue engineering industries. Current research in tissue engineering focuses on utilizing the micro-environment of scaffolds to guide cell function. While scaffolds are intended to support viable cells, validated methods of measuring cell viability within scaffolds are not available in the public domain. We are developing model scaffold-cell-assay systems for assessing viability measurements. Collagen is used for the scaffold, since this is the most widely used extracellular matrix system for 3D cell encapsulation. Highly purified collagenases are available to release viable cells from scaffolds to confirm results from assays conducted on cells in situ. An ATP luminescence assay is used, since intracellular ATP is a good indicator of viability. The Jurkat cell line has stable performance, is widely available, and is well-studied. Encapsulation protocols have been evaluated to find a robust and reliable protocol that yields cells with high levels of intracellular ATP. The following factors have been assessed: composition of encapsulation medium, ionic strength, pH, gel fraction, and gelation time. The collagen scaffold system can efficiently encapsulate Jurkat cells. To release the cells from the scaffold, collagenase effectively breaks down the collagen. ATP spike-in experiments showed that ATP could be reliably measured in situ within intact collagen gels. ATP spike-in experiments also showed that ATP could be reliably recovered from collagen gels using the collagenase digestion. Control experiments were conducted to show that collagenase did not harm cells. Cell viability within the scaffold was measured using the ATP assay, however, unpredictable pH variation resulted in fluctuating cell viability. Developers of tissue engineered medical products can benefit from detailed protocols for conducting and validating measurements of cell viability in scaffolds.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Klara Keim		
Academic Institution: Texas Tech University	**Major:** Microbiology	
Academic Standing (Sept. '19):	First Year Ph.D. Student	
Future Plans (School/Career):	I am pursuing a Ph.D. in Microbiology at the University of Colorado for future work in bacteriology and infectious diseases research.	
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group	
NIST Research Advisor:	Dr. Stella Alimperti	
Title of Talk:	Elucidating the Effect of Extracellular Matrix Stiffness in Oral Microvasculature Utilizing Microfluidic Devices	

Abstract:

Oral microvascular diseases are strongly correlated to other diseases, such as oral cancer, hyperglycemia-induced periodontitis, and diabetes, which have traumatic effects on the soft tissue surrounding oral microvessels. These diseases affect the stiffness of the extracellular matrix (ECM), which acts as a scaffold for endothelial cells comprising the microvasculature. Ultimately, this alters characteristics important in maintaining the growth and integrity of vessels, including cellular growth, adhesion, cytoskeletal arrangement, and translocation of components, such as the Forkhead Box Protein O1 (FOXO1), important in regulating metabolism, proliferation, and angiogenesis of the microvessels. The current research focuses on developing a microfluidic platform allowing for quantification of the effects of ECM stiffness on the integrity of the oral microvasculature, including cytoskeletal characteristics and the cytonuclear translocation of FOXO1. In this study, we fabricated microfluidic devices in polydimethylsiloxane (PDMS) and seeded human umbilical vein cells (HUVECS) into a cylindrical collagen matrix to recapitulate proper 3D oral microvascular structures. The engineered vasculature was then utilized to observe physiological responses to varying conditions of collagen matrix stiffness. We engineered a 3D ECM using concentrations of type I collagen ranging from 1 mg/mL (softest matrix) to 4.2 mg/mL (stiffest matrix). Confocal microscopy was then utilized to visualize and quantify alterations in permeability of the vessel, cytonuclear translocation of FOXO1, and cytoskeletal rearrangement in response to the stiffness of the ECM. We have shown that a softer matrix decreases vessel integrity, exhibiting increased permeability and diffuse cytoskeletal arrangement around the cells. Whereas, in a stiffer matrix, the vessel exhibits decreased permeability and the cells exhibit increased spreading of their cytoskeletal elements. Additionally, FOXO1 has been observed to be translocated into the nuclei of the cells. The impact of this work elucidates the physiological effect of varying ECM stiffnesses resulting from a diseased environment. For example, the oral microvascular environment in patients with diabetes shows increased glucose levels, expression of inflammatory cytokines, and reactive oxygen species leading to tissue damage, in addition to stiffening ECM, which ultimately leads to impaired wound healing. Therefore, this study will allow for an efficient multiparametric model to quantify the effects of stiffening ECM on the microvasculature, elucidate potential therapeutic methods, and advance methods of vascular tissue engineering for *in vivo* and *in vitro* applications.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Eleanor Kelman		
Academic Institution: Brandeis University	**Major:** Computer Science, Linguistics, Hispanic Studies	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Graduate school for Computer Science or Computational Linguistics	
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division,	
NIST Research Advisor:	Dr. Aaron Gilad Kusne	
Title of Talk:	Finding High Conductive Transparent Oxides with Active Learning	

Abstract:

Active learning is the subset of computer science in which a computer learns about possible experiments and independently chooses which one to perform next to reach a desired goal. Active learning algorithms are useful because they save time and resources when running real-world experiments. Since every possible experiment cannot feasibly be performed, the selected algorithm can reduce the number of experiments by selecting the preferable one at every iteration of the code to reach an optimal solution sooner than if every considered experiment were to be performed.

Exploration of active learning optimization was performed on a set of simulated data points using Gaussian process for regression, along with tests to quantify performance of the algorithms. This understanding of active learning algorithms is then applied to real-world problems, particularly experimentation involving the conductivity of transparent oxides.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Jinsung Lee		
Academic Institution: Johns Hopkins University	**Major:** Chemical and Biomolecular Eng.	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Graduate School/Researcher	
NIST Laboratory, Division, and Group:	MML- Material Science	
NIST Research Advisor:	David Raciti	
Title of Talk:	Determining Optimal 3-D Configuration of Porous CO2 Reduction Catalysts	

Abstract:

Increasing levels of atmospheric CO2 in the past century due to human consumption of fossils fuels is strongly correlated to drastic changes in the global climate. One proposed solution, to alleviate increasing CO2 levels and global reliance on fossil fuels is the electrochemical reduction of CO2 to useful commodities such as ethanol or carbon monoxide. However, the efficiency of this process is likely limited by non-optimal configurations of fabricated catalysts. This study aims to discover the relationship between porous catalyst thickness and output of a CO2 electrolyzer. We propose that an optimum thickness will maximize CO2 diffusion through available active sites enabling maximize utilization of supplied carbon dioxide and favor the conversion of CO2 into desired products. For instance, thinner catalysts may not fully utilize the CO2 diffusing through the pores, while thicker catalysts' active sites may not be saturated with enough CO2 thus encouraging parasitic H2 evolution.
We prepared porous catalysts through a hydrogen-evolution assisted electrochemical deposition. In this method, a target metal (Cu or Ag) is deposited onto a hydrophobic gas diffusion layer. To do this, an applied potential is held where hydrogen gas evolution and metal deposition occur simultaneously, which allow the hydrogen bubbles produced to serve as a template for pore formation. By controlling the duration of deposition, the thickness of the resulting foam-like macrostructure can be tuned. From scanning electron microscopy (SEM), we have resolved dendritic-like branches at nanoscale and spherical micro-porosity, which stems from the hydrogen bubbles during deposition. Additionally, cross-sectional SEM enabled determination of catalyst thickness.
Following fabrication, each catalyst was tested in a custom-built gas diffusion electrode where the gas products are analyzed in-operando with gas chromatography. The results from these studies draw correlations between conversion rates of CO2, selectivity towards CO2 reduction (vs H2 evolution) and overall current densities based on catalyst thickness. Additionally, it expresses the importance of evaluating 3-D features and microscopic structure of potential catalysts. In further studies, we seek to simulate and further tune the microporous structure of the catalyst to both advance our understanding of and improve the transport of CO2 through the catalyst.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2018

Name: Simin Manasiya		
Academic Institution: University of Houston		**Major:** Biomedical Engineering
Academic Standing (Sept. '19):	Graduated	
Future Plans (School/Career):	Graduate School	
NIST Laboratory, Division, and Group:	MML, Materials Science and Engineering Division, Functional Polymers Group	
NIST Research Advisor:	Dr. Frederick Phelan, Jr.	
Title of Talk:	Using Atomistic Simulations to Relate Local Molecular Dynamics and Fluorescence Lifetime in a Damage Sensing Dye	

Abstract:

Polymer composites are a class of materials composed of a matrix and a reinforcement phase which is often constructed from fibers. Around the vicinity of the fiber, where the matrix properties begin to vary from those in the bulk, is called the interphase and the point where the matrix and fiber meet is the interface. Together these regions are responsible for providing rigidity and overall strength to the composite. Mechanical or water damage, which is characterized by change in interface level chemistry or phase separation, often occurs at this region with the consequence of failure of the overall composite and its mechanical properties.
Fluorophores are molecules that absorb photons to attain an excited state and emit light as they transition to a lower energy state during a process called quenching. Fluorescent lifetime is the amount of time a molecule spends in the excited state before returning to ground state and is a function of the dye molecule chemistry and its surrounding environment. NIST is developing a type of fluorophore called a mechanophore that attains an excited state upon covalent bond breakage at the interface level and subsequently fluoresces. These mechanophores, when embedded at the interface level, can function as damage indicators for composites if the mechanical strain becomes too great.

In this project, we use molecular dynamics to study a fluorescent dye in different molecular environments for quantifying its dynamics which correlate with fluorescent lifetime in potential mechanophores. The dye we study is Rhodamine B which exists in a conjugated state and fluoresces at a 610 nm. An environment with higher solvent viscosity generally yields a greater fluorescence lifetime; this is desirable for a better signal detection in tests of composite damage. Therefore, we studied the behavior of Rhodamine B in several solvents and attempt to correlate the dihedral relaxation function of the conjugated nitrogen atom with experimental results for the lifetime changes measured in solvents of different viscosity. Molecular Dynamics (MD) simulations provide a realistic and inexpensive way of studying molecular behavior with a wide array of desired environments. We perform MD simulations on several Rhodamine B molecules in a variety of solvents with differing viscosities and study the dihedral bonds that allow it to fluoresce. As expected, the preliminary results indicate that the dynamics of the molecule do tend to change with viscosity. These protocols will assist in the development of experimental designs of similar fluorogenic compounds and mechanophores.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Joelle Marchiani		
Academic Institution: Hawai'i Pacific University		**Major:** Marine Biology
Academic Standing (Sept. '19):	Masters Student, Northeastern University	
Future Plans (School/Career):	I'm attending graduate school for a M.S. in Marine Biology, and my goal is to work as a Laboratory Assistant or Research Technician	
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Environmental Chemical Sciences Group	
NIST Research Advisor:	Jennifer Lynch	
Title of Talk:	Chemical weathering and additives in plastic marine debris in the Hawaiian Islands	

Abstract:

Marine plastic pollution is a growing issue, and researchers need best methods for quantifying and characterizing plastic in complex environmental samples. Weathering of plastic polymers leads to the leaching of additives into the environment which potentially have detrimental health effects. The three main objectives of this study were to: (1) mine existing attenuated total reflectance Fourier transform infrared (ATR FT-IR) spectra of Hawaiian marine debris for polymer additives, (2) mine existing spectra for a carbonyl band which is indicative of photo-oxidative weathering and (3) conduct an outdoor natural sunlight weathering experiment to determine when a carbonyl band develops. For objective 1, spectra of 37 samples of Hawaiian marine debris (out of ~3500) show strong phthalate additive bands. Future spectral library searches will attempt to identify the phthalate compound, and determine whether FT-IR is an effective technique for identifying presence of additives in Hawaiian marine debris. For objective 2, the carbonyl band could potentially be used to aid in aging littered plastics. Preliminary results on nine samples suggest that carbonyl bands are not stronger for the most weathered Hawaiian PE or PP samples; however, future analysis of the external surface of the debris (rather than clean internal surface) and an increased sample size will improve this assessment. For our outdoor weathering experiment, three replicates of six polymer standards were placed on a glass surface over sand in direct sunlight in Waimanalo, Oahu, Hawaii: polyethylene terephthalate (PET), high density polyethylene (HDPE), low density PE (LDPE), polypropylene (PP), polystyrene (PS), and polylactic acid (PLA). Polymers placed alongside these in darkness served as controls. Preliminary results from the weathering experiment indicate there were no statistically significant changes in mass in the first 18 days for the 6 polymer types. No carbonyl bands formed, and no visual changes to the polymer surfaces were apparent under a dissecting microscope. Future time points will determine when plastic debris develops a detectable carbonyl band.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Oriana Christy Ovide		
Academic Institution: West Virginia University	**Major:** Forensic Science and Chemistry	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	I would like to work as a forensic chemist after attending graduate school	
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Division 643, Group 2	
NIST Research Advisor:	Ruthmara Corzo, PhD	
Title of Talk:	Assessment of Elemental Homogeneity in Modern Glass µXRF for Forensics	

Abstract:

The widespread use of glass in everyday items contributes to its importance in forensic science. Glass is a type of trace evidence that can be found at various crime scenes such as hit-and-runs, homicides, and burglaries. Glass is particularly beneficial to forensic science because small fragments can easily be transferred during the commission of a crime and are fairly persistent. Soda-lime float glass (e.g., architectural and automotive windows) is the most common type of glass encountered in forensic casework. The major components of soda-lime glass are kept relatively consistent by manufacturers, however leaching from the production process and trace impurities in the raw materials result in elemental differences between glass produced by different manufacturers and between production batches within a manufacturing plant. These differences in elemental composition are useful for differentiating glass fragments from different sources; similarly, the absence of elemental differences is indicative of a potential common origin. Micro x-ray fluorescence spectroscopy (µ-XRF) is the most commonly used technique for the elemental analysis of glass in forensic casework. With µ-XRF's growing usage comes the need for research assessing the homogeneity of a single glass source. In this study, 50 glass fragments were each collected from the inner and outer glass panes of a single windshield. The fragments were analyzed using µ-XRF, and the relative standard deviation (RSD) was calculated to evaluate the homogeneity within a single glass. The outer pane was found to be fairly homogenous for all elements detected (RSD< 10%), apart from titanium and sulfur. The inner pane exhibited greater heterogeneity (RSD > 15%), though this is in part attributed to x-ray scattering caused by irregular surfaces. The homogeneity within a glass source has important implications for proper sampling to ensure that the known fragments collected from a crime scene are representative of the glass source.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Rajashow Parajuli		
Academic Institution: Montgomery College	**Major:** Computer Science	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Graduate school or career in swarm intelligence	
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science & Engineering Di	
NIST Research Advisor:	Dr. Debra Audus	
Title of Talk:	Predicting Protein Properties with Machine Learning	

Abstract:

Proteins are life essential biological molecules composed of chains of bonded amino acids. Its amino acid sequence dictates each protein's unique structure, behavior, and properties. The combinations of the twenty naturally occurring amino acids are responsible for maintaining, creating, and defending all biological processes. In structural and chemical biology, proteins' behaviors are used in drug discovery and gene therapy, which has improved the lives of patients suffering from disease like sickle cell anemia, hemophilia and cancer. However, The most common methods of predicting protein's material properties involve expensive experiments or using simulation on already predetermined 3D structure of a protein. Furthermore attempting predicting protein behavior from its sequence by hand or computationally is a nontrivial endeavor due to cross interactivity of amino acids with each other. The ability to predict properties for any given sequence would reduce the experimental effort and would allow for rapid prototyping of material samples for testing. We have used existing sequenced proteins and their respective structures found in open protein databases such as the Protein Data Bank with machine learning methods to predict protein properties.We tested machine learning methods from simple methods as linear regression to complex models like random Forests, Multi-layer, and Convolutional neural networks with a different representation of the sequences such as one hot encoding, a bag of words and correlation matrix. We have benchmarked proficiency of each machine learning method in predicting crystalline protein's material properties such as volume, hydrodynamic radius, intrinsic viscosity, and gyration and polarizability tensors.In addition, we have found that the neural networks not only outperform but also the performance scales with data.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Samuel Philliber		
Academic Institution: California Polytechnic State University	**Major:** Physics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Pursue a PhD in physics	
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, The Ma	
NIST Research Advisor:	Dr. David LaVan	
Title of Talk:	Developing a Virtual Instrument for a High-Throughput Thermal Analysis Instrument	

Abstract:

Picocalorimetry allows for the measurement of the thermodynamic properties of nanoscale samples. Larger datasets are desired for further analysis of melting points, heat capacity, enthalpies, etc.; however, current instrumentation can only accommodate one sample at a time; measuring less than ten samples a day is normal. This new instrument is intended to measure thousands of samples a day. Each sample must be aligned under a detector, which will be done using machine vision and automated stages to move between multiple samples on a single wafer and then perform a thermal measurement using optical methods. In order for this new instrument to run, each of its components need to be controlled through a single program - the camera, the stages, the 1550 nm interferometer, the 980nm heating laser, etc.

I will report on the progress in the development of the LabView code to coordinate the operation of the stage motors and the interferometer. With these working together, the instrument can now be tested and some data can be taken. The program also processes, analyzes, and stores the interferometer data from each sample. Future work is to get the built-in mass-spectrometer running.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Joshua Price		
Academic Institution: The Pennsylvania State University	**Major:** Biology	
Academic Standing (Sept. '19):	Post-baccalaureate	
Future Plans (School/Career):	National Institutes of Health's IRTA program and pursue a doctorate degree.	
NIST Laboratory, Division, and Group:	Material Measurements Laboratory, Biomolecular Measurement Division, Biomolecul	
NIST Research Advisor:	Zvi Kelman, William Brad O'Dell	
Title of Talk:	Calibrating Deuterium Incorporation into Green Fluorescent Protein Expressed in the	

Abstract:

Stable isotopic labeling, in which atoms of a molecule at natural isotopic abundance are replaced with one or more specific, non-radioactive isotopes, is a powerful technique for creating chemically-similar but isotopically-distinguishable materials for study by methods such as mass spectrometry, nuclear magnetic resonance (NMR) spectroscopy, and neutron scattering. Within biology, deuterium labeling of proteins and other biomacromolecules can enable detailed studies of molecular structure and dynamics which underpin biological function. While deuterium incorporation into proteins utilizing prokaryotic expression hosts has been relatively well defined, eukaryotic proteins cannot always be expressed by prokaryotes, creating a need to improve upon current methods. Thus, the intent of this project was to utilize the yeast Komagataella phaffii (K. phaffii) to create a calibration curve for the incorporation of deuterium into the model protein green fluorescent protein (GFP) as a function of deuterium substitution in the growth medium. This was accomplished by transforming K. phaffii to express GFP upon methanol-dependent induction, growing K. phaffii in variably deuterated media, purifying the expressed GFP, and measuring deuterium incorporation using matrix assisted laser desoprtion/ionization (MALDI) mass spectrometry. As expected, GFP deuterium incorporation increased monotonically, but non-linearly, as a function of the deuterium content of the medium used for growth, and the addition of a deuterated carbon source was necessary to approach full deuterium substitution (perdeuteration). These experiments are the first effort to calibrate deuterium incorporation by K. phaffii and provide useful reference data for future projects where specific levels of deuterium incorporation into proteins by K. phaffii is required.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Adam Robinson

Academic Institution: George Mason University | **Major:** Physics

Academic Standing (Sept. '19): Senior

Future Plans (School/Career): Graduate school (PhD in Physics)

NIST Laboratory, Division, and Group: MML (63) (Division=642)(Thermodynamics and Kinetics Group (642.05))

NIST Research Advisor: Dr. James Hickman

Title of Talk: Neural network interatomic potentials: Feature selection and property sensitivity

Abstract:

In order to carry out realistic classical atomistic simulations it is essential to have an accurate mapping between a system's atomic structure and its potential energy. The function that describes this relationship is known as the potential energy surface (PES). The PES can be estimated using various computationally slow but highly accurate quantum mechanical methods such as density functional theory (DFT). Alternatively, faster but less accurate physically inspired analytic models are also common. Collectively, analytic approximations of the PES are known as interatomic potentials or force fields. In recent years artificial neural networks (ANN) have also become popular as a means of predicting energy by interpolating DFT data. The ANN approach requires the quantification of a given atom's local structural environment by a descriptor vector (also known as a feature). This vector is fed into the ANN which can be trained using DFT data to make a prediction for the atom's potential energy. The ANN method approaches the accuracy of DFT but is computationally much faster. In the present study we apply common machine learning feature selection algorithms to determine the feature sets which strike the optimal balance between computational speed and accuracy. We focus on silicon as a model system; however, generally the results apply to any mono-atomic system. Finally, using this optimal set of features, we demonstrate convergence of various thermal properties with respect to how tightly a given ANN force field reproduces the results of DFT.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Katrina M Rupert

Academic Institution: West Virginia University | **Major:** Forensic & Investigative Science

Academic Standing (Sept. '19): First year Graduate Student, B.S. in Forensic & Investigative Science

Future Plans (School/Career): Graduate school for Forensic Biology at WVU

NIST Laboratory, Division, and Group: MML, Division 645, BioProcess Measurement Group

NIST Research Advisor: Jeffrey Hudgens & Kyle Anderson

Title of Talk: Getting the Kinks Out: Reducing Disulfide Bonds for Protein Analysis

Abstract:

In order to sell viable medications to the public, biopharmaceutical companies must fully comprehend how each medication interacts with the target protein in the human body. A prominent instrument utilized to analyze the functionality of proteins in their "holo-" and "apo-" configurations is hydrogen-deuterium exchange mass spectrometry (HDX-MS). Hydrogen deuterium exchange ultimately reveals the flexibility of proteins. Following a period of HDX protein flexibility is evaluated by digesting the protein into peptides and then measuring the deuterium content of each peptide. HDX-MS has been applied to determine the mechanism of action of candidate treatments for various medical conditions including diabetes, Alzheimer's and cancer. However, an obstacle to this method is the presence of disulfide bonds as they inhibit and complicate analysis. A common chemical process applied to aid in the reduction of these bonds is TCEP, yet the process proves ineffective on many proteins and on some instruments. A novel electrochemical device advertised to be successful in disulfide reduction for a wider array of proteins is Antec's μ-PrepCell 2.0.

This summer's project focuses on validating the μ-PrepCell, optimizing various parameters for the best reduction of different samples, as well as attempting to incorporate the cell into the HDX-MS workflow. Antec exemplified the success of their cell by working with insulin so verifying the cell reduces a sample within water was the first step to take. The cell was isolated with just a liquid chromatograph mass spectrometer to complete the verification. Once sample reduction in water was achieved, the question arose if the cell could still perform on a sample when combined with a salt at physiological concentrations. Variables evaluated consist of flow rate, voltage and length of each pulse, salt concentration. If disulfide reductions can be achieved on a sample prepared for HDX, the cell could feasibly be incorporated into the HDX-MS workflow to aid in the analysis of proteins previously inhibited by disulfide bonds.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Usmaan Siddiqui		
Academic Institution: University of South Florida	**Major:** Chemical Engineering	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Graduate School in Chemical Engineering	
NIST Laboratory, Division, and Group:	MML, MSED, Polymers Processing Group	
NIST Research Advisor:	Daniel Sunday	
Title of Talk:	Self Assembly and Solution Structure of Supramolecular Bottlebrush Polymers	

Abstract:

Supramolecular polymers are unique compared to traditional polymers in that they are composed of key reversible and directional secondary bonding. Secondary bonds, most notably hydrogen bonds, can be finetuned and can consequentially alter the polymer's material properties. Studies on self-assembly typically use short small molecules for hydrogen bonding, yet it is unclear how well short polymers (<5k Daltons) will assemble. To study the impact of how sidechain length impacts supramolecular assembly, hydroxyl terminated polystyrene (PSOH) sidechains were grafted onto a poly-4-vinylpryidine (P4VP) backbone. P4VP was chosen as the backbone due to the strength of the pyridine groups as an H-bond acceptor while PSOH of varying molecular weights were used as the pendant chains. Fourier-Transfer Infrared Spectroscopy (FTIR) was primarily used to investigate the hydrogen bonding occurring in the bottlebrush samples. Employing FTIR methods provides fundamental results in analyzing the amount of pyridine groups in P4VP that are participating in supramolecular self-assembly.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Noah Smith		
Academic Institution: Drake University	**Major:** Chemistry, Physics, & Mathematics	
Academic Standing (Sept. '19):	Graduate Student	
Future Plans (School/Career):	Master's in Chemical Engineering at Washington University in St. Louis	
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials for Energy and Sustainable Development	
NIST Research Advisor:	Dr. Zachary Trautt	
Title of Talk:	Enabling FAIR Data Principles for High-Throughput Experimental Data	

Abstract:

In materials science and engineering, the ability to generate and process data has increased tremendously in recent years, but storing, sorting, and managing data has remained an ongoing challenge. To aid in developing an infrastructure to manage data repositories scientists and engineers are embracing the FAIR Data Principles. The FAIR Data Principles advocates to make data Findable, Accessible, Interoperable, and Reusable. Additionally, they focus on the ability of machines to find and use datasets to further increase the usability of data in any field. However, computers and humans interpret and process information very differently and therefore web services need to be developed with both in mind.

The needs of computers and humans to process information are starkly different. Computers need data in a well-structured format. This is accomplished by using Cordra, a software tool that can enable FAIR data principles throughout the data lifecycle. To satisfy the needs of human's, web services need to be intuitive, interactive, and enable visualization of the data. Visualization of the data enables data consumers to quickly decide if they want to spend more time downloading and using the data. Creating these interactive web services and visualizations of high-throughput experimental materials data is the focus of this SURF project. This is accomplished by utilizing JavaScript and libraries like D3.js in conjunction with HTML and CSS.

JavaScript is leveraged to keep the webpage and visualizations clean and distinct from the base HTML coding and CSS styling. D3.js is a specific JavaScript library that focuses on making documents data driven which allows for much more responsive webpages and visualizations. With the help of Cordra, the data and metadata can be accessed through a REST API allowing for much greater interoperability between data sets.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Ryan Smith
Academic Institution:	University of Houston
Major:	Chemical Engineering
Academic Standing (Sept. '19):	Graduate Student
Future Plans (School/Career):	I plan to earn my Ph.D. in Chemical Engineering at Notre Dame
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Materia
NIST Research Advisor:	Dr. Jason Hattrick-Simpers
Title of Talk:	Correlating Structural and Functional Properties with Amorphicity of Alloys.

Abstract:

Metallic glasses (MG), also known as amorphous metals, are technologically interesting 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. Previously at NIST, a particularly interesting alloy system, NiTiAl, was predicted by machine learning models to form a glass in a composition region that should not yield a stable glass according to traditional heuristics. This system was then synthesized as a thin film and investigated for its MG forming ability through synchrotron x-ray diffraction. Comparison of an alloy's x-ray diffraction peak full width at half maximum (FWHM) value with those of known glasses is a convenient way to determine whether that alloy is a glass, but the precise FWHM threshold that qualifies an alloy as a glass is ambiguous. As a result, the full extent of the glass-forming composition region was difficult to precisely quantify and compare to the machine learning predictions. Since MG alloys can (though do not necessarily) exhibit much higher corrosion resistance than crystalline alloys, this study aimed to correlate corrosion properties with the FWHM and alloy composition. The corrosion properties, such as passivation current, of the NiTiAl system were measured with a scanning droplet cell on a NiTiAl composition gradient thin film deposited on a silicon wafer. Correlating those results to composition and FWHM illustrated that a FWHM value greater than approximately 0.42 Å^-1 was necessary but insufficient for any given composition to exhibit high corrosion resistance. Using this new threshold value, it was determined that the glass forming region of the NiTiAl alloy system is significantly larger than previously believed. Future application of the FWHM threshold to other systems could reveal currently undiscovered or unpredicted metallic glass systems or composition regions.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Lu Song
Academic Institution:	Pennsylvania State University
Major:	Material Science and Engineering
Academic Standing (Sept. '19):	Senior
Future Plans (School/Career):	Continuing school and pursuing a career in Material Science and Engineering area
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory (MML), Material Science and Engineering Division (MSED), Polymer Processing Group
NIST Research Advisor:	Anthony Kotula
Title of Talk:	Evaluating mechanical and chemical properties of polydimethylsiloxane using rheo-Raman microscope.

Abstract:

Polymer cross-linking results in the modification of mechanical properties due to the formation of covalent bonds between polymer chains, which significantly impacts processing conditions used to produce industrial products. Polydimethylsiloxane (PDMS) has been widely used in industrial products due to its viscoelastic and transparent properties, non-toxicity, and non-flammability. The goal of the present work is to determine the relationship between the extent of reaction and resulting viscoelastic properties of PDMS using the rheo-Raman microscope. The rheometer is used to investigate the mechanical properties (viscosity and shear modulus) of PDMS during isothermal cure conditions. For each experiment, dynamic frequency sweeps are performed to monitor the increase in the viscosity and modulus. These viscoelastic properties are used to determine when rheological transitions from liquid-like to solid-like material occur. Raman spectroscopy is used to examine vibrational modes that participate in the cross-linking reaction with adequate peak resolution as the polymer solidifies. Peaks associated with Si-H and C=C vibrational modes decrease in intensity since the bonds form the cross-link, but these peaks have a low signal-to-noise ratio. Through calculating the peak height ratio of C-H stretch modes that evolve during the reaction, the cross-linking process can be monitored over time at various temperatures. The extent of reaction can be estimated through the peak height ratio and fit using the autocatalytic model to determine the effect of temperature on the cross-linking kinetics. By combining both rheology and Raman spectroscopy analysis, the shear modulus can be plotted versus the extent of reaction to show the sensitivity of mechanical properties to the extent of the cross-linking reaction at different cure temperatures. The current analysis of combining rheo-Raman data is used to test the accuracy of existing rheological models to estimate the extent of reaction.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Jonah Tash		
Academic Institution: University of Maryland, College Park	**Major:** Computer Science & Math	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Graduate School/ Industry	
NIST Laboratory, Division, and Group:	MML, Biosystems and Biomaterials Division, Cell Systems Science Group	
NIST Research Advisor:	Dr. Talapady N. Bhat	
Title of Talk:	Dynamic Taxonomies for Root & Ruled Based Language Trees	

Abstract:

Taxonomies are an intuitive way of structuring large corpora of data. They can be used to organize research institutions, organisms, and even the words in this abstract. The basic structure of a taxonomy is a tree with branches representing nested categories. Taxonomies are valuable to researchers because this structure quantifies data similarity. For example, one might expect humans to share more characteristics with primates than reptiles since humans belong to the primate taxonomic class. Furthermore, this feature would be valuable to an online retailer using a taxonomy to organize their products. A user interested in a specific item might also show interest in items from the same taxonomic family. The store can suggest these items to the user, keeping that shopper on their website for as long as possible. There is a disadvantage to using taxonomies in this manner. The only way to find an item is by searching every branch of the tree until the desired item is found. We developed dynamic taxonomies solve this inefficiency. In a dynamic taxonomy, entries are stored in a flat table. Taxonomic classes are defined not by explicit branches, but as shared characteristics between elements. This allows classes to be created dynamically. This concept was implemented as a webapp using the C# ASP.NET framework. The app allows users to build their own abstracts using snippets from other papers. As users search for snippets, the app displays search suggestions generated by the Root & Rule (R&R) processing method. The R&R method distills keyword-like phrases from the documents. Users can then choose to add the phrase as a taxonomic characteristic to help refine their search. The app was a successful proof-of-concept for this new technique. This work is a starting point for future research on dynamic taxonomies.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Winnie Tran		
Academic Institution: University of Maryland College Park	**Major:** Biochemistry	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Pursuing either a career in Biochemistry field, or a Master's Degree in Biochemistry	
NIST Laboratory, Division, and Group:	MML, Biomolecular Measurement Division, Bioanalytical Science Group	
NIST Research Advisor:	David M. Bunk	
Title of Talk:	Combining LC-MS and ELISA for Quantification of Allergenic Milk Protein in Food	

Abstract:

The prevalence of food allergy has become an important public health issue and economic concern to the U.S population. As there is no cure or preventative treatment currently available, the best way to avoid food allergy exposure is strict dietary avoidance. The U.S 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 in 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-contact, 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 to quantify protein allergens in Nonfat Dry Milk 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 the future, the method created from this project will be combined with commercial immunoassays (ELISA format). We will evaluate both qualitative and quantitative measurements of the digested ELISA samples through LC-MS/MS analysis.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Nidhi Vantair		
Academic Institution: Johns Hopkins	**Major:** Neuroscience	
Academic Standing (Sept. '19):	Graduate Student	
Future Plans (School/Career):	Georgetown University/ Medicine	
NIST Laboratory, Division, and Group:	MML, Biosystems and Biomaterials Division, Complex Microbial Systems Group	
NIST Research Advisor:	Dr. Scott Jackson	
Title of Talk:	Developing a Candidate Reference Material to Assess DNA Extraction Efficiency	

Abstract:

In the past decade, the human microbiome has been linked to a plethora of health and disease conditions. The advent of new DNA sequencing technologies (so-called Next-Generation Sequencing or NGS) have recently provided us with the tools necessary to classify these various bacterial communities. In doing so, we can characterize which microbial compositions are encompassed by healthy individuals and diseased individuals. Any abnormalities in health and microbiome composition can thus be potentially linked together. Most microbiome composition measurements are NGS-based and thus necessitate a DNA extraction step. There are currently many different types of NDA extraction methods; however, none are 100% efficient methods across all cell types. To understand the extent of bias introduced by DNA extraction, we set out to create a standard that assesses the extraction efficiency of various methods.

Saccharomyces cerevisiae is a model organism and is notoriously difficult to lyse because of its sturdy cell wall. While it is instrumental in baking and brewing, our hope is to use it to develop an engineered strain of yeast that has marker genes from bacteria. the engineered yeast will contain synthetic 16s genes that are uniquely identifiable among the rest of the bacteria. NIST has previously developed validated procedures for quantifying yeast cells. With a known amount of genetically-engineered yeast cells placed into the samples of microbiome communities, we can conduct the extraction methods to measure how efficient each method is based on how much of the synthetic yeast 16s genes are recovered. By using this material as a spike-in to assess DNA extraction efficiency, these yeast cells can be utilized as a reference material to detect bias within research and ultimately link microbiome abnormalities with human disease conditions.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Yuke Wang		
Academic Institution: University of Kentucky	**Major:** Physics, Math, Computer Science	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Graduate school for Physics PhD	
NIST Laboratory, Division, and Group:	Material Measurements Laboratory, Polymer Division, nSoft Group	
NIST Research Advisor:	Tyler Martin	
Title of Talk:	Feature Engineering for Small Angle Neutron Scattering A.I	

Abstract:

Small-angle neutron scattering (SANS) is a technique used to measure the thermodynamic and structural properties of materials. In SANS, a neutron beam interacts with a material and produces a scattering pattern depending on the nanostructure of the material. However, finding correlations between scattering patterns and material properties is difficult as the patterns produced by different structures are not linearly separable and the noise and smearing of detectors further obfuscate the data.
Machine learning and artificial intelligence (ML/AI) offer the promise of revolutionizing many scientific data tasks, including the interpretation and processing of scattering data. Unfortunately, due to the cost and slow acquisition time from SANS measurements limited data is available. This means applying some of the most powerful ML/AI techniques (e.g., deep learning) is not feasible and training traditional classifiers on the raw data results in very low accuracy. The specific goal of this project is to engineer a set of features used as inputs for ML/AI algorithms to extract useful information from small SANS data sets and, furthermore, to identify the most important features for extracting specific materials properties. To achieve this goal, we are considering several feature creation methods: manual feature engineering, automated feature selection, and transfer learning. Some engineered features will be physics based, such as identifying power law scaling regions and scattering peaks. Automated feature selection involves creating a large number of features procedurally, then using an algorithm to determine the most important features. Deep nets can also be trained on simulation data, then the feature outputs from the first fully connected layer can be used as inputs to non-deep classifiers to fit new data. By comparing and potentially combining these methods, we will develop protocols for building robust scattering classifiers and regressors. This project is contributing to a larger effort develop a ML/AI toolset for scattering with the ultimate goal of partially automating the process of analyzing and interpreting SANS data.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Gamitha Wijekoon		
Academic Institution: University of Maryland, College Park	**Major:** Mechanical Engineering	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Masters Degree in Robotics Engineering	
NIST Laboratory, Division, and Group:	MML, 646.05	
NIST Research Advisor:	Dr. Heather Chen-Mayer	
Title of Talk:	Neutron Tomography and Simulation of Compton Imaging	

Abstract:

With the aging infrastructure in America, we need to be able to assess the condition of infrastructure while it is in use. Current methods allow one to determine the structural and material composition of a sample but destroy the sample in the process. My research focuses on using Neutron Tomography and Compton Imaging to determine structural and material composition of a sample without destroying it.

We currently use Prompt Gamma Activation Analysis (PGAA) which gives us information on the materials of the sample but we do not know where in the sample the materials are. Neutron tomography allows us to map the structure of a sample, however, we do not gain much information about the material composition of the sample. We hope to extend the capability of PGAA by implementing Compton Imaging of the prompt gamma rays because it tells us what is in the sample and where it is with decent accuracy. I implemented a simple Neutron Tomography system at the PGAA facility using a camera and xyz and rotational stage which I interfaced together and wrote control code for in LabVIEW to automate the Neutron Tomography process. Using that system, we hope to do Compton imaging reconstruction in 3D faster and with higher accuracy. We are currently in the process of designing a Compton imaging setup using the Geant4 Simulation software by CERN. By varying certain parameters of the setup such as detector spacing and pixel size and running the simulations, we can continue to iterate our design until we find a setup that meets the imaging characteristics we would like.

My work currently uses a reactor to provide neutrons for PGAA and Neutron Tomography. We hope in the future that portable neutron sources can be used to inspect infrastructure using Compton Imaging and Neutron Tomography.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Fjorela Xhyliu		
Academic Institution: Cleveland State University	**Major:** Chemical Engineering	
Academic Standing (Sept. '19):	Graduate Student	
Future Plans (School/Career):	Graduate Degree in Biomedical Engineering	
NIST Laboratory, Division, and Group:	MML, Material Science and Engineering Division, Polymers and Complex Fluids Group	
NIST Research Advisor:	Gil Kaufman (Advisor), Jonathan Seppala, Anthony Kotula	
Title of Talk:	NAC rescues dental pulp cells exposed to toxic dental monomer	

Abstract:

Dental pulp regeneration and its biomineralization functions are affected by various factors such as the exposure to toxic monomers leaching from nearby restorations. One approach to preserve the pulp tissue is to induce the deposition of tertiary dentin mineral as a protective layer. In this study, we: 1) identify the measuring tools to follow development and accumulation of hydroxyapatite (HA) mineral deposited by dental pulp cells (DPCs)/microtissues in extracellular matrix (ECM), 2) determine the capability of multifunctional rescuing drug, n-acetyl cysteine (NAC), to recover/resume the biomineralization of DPCs exposed to triethylene glycoldimethacrylate (TEGDMA), and 3) compare the effect on biomineralization of NAC conjugated to HA and/or dicalcium phosphate anhydrous (DCPA), i.e., HA/DCPA-NAC particles vs. the inductive particles conjugated to lipid derivatives. 2D and 3D primary human DPCs were evaluated through Raman micro-spectroscopy for the production of HA particles. Relative change in the HA particles concentrations was established for NAC-treated vs. non-treated conditions. Mineral imaging/Alizarin red assays were employed to visualize the spatial organization and deposition of the HA particles and validate the amount of the mineral. NAC allowed a continuous development of the dental pulp microtissues and prevented matrix mineralization in the absence of TEGDMA. However, upon the exposure to toxic concentration of TEGDMA (1.5 mmol/L), NAC was required to resume the biomineralization. The effect of the NAC-conjugated to HA and DCPA particles is currently being investigated. To-date results suggest that NAC could be clinically utilized as rescuing agent incorporated into pulp-capping restoratives or bio-printed into multifunctional organic matrixes that will allow cells to regenerate and induce biomineralization when affected by toxic dental monomers.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Julie Yagodich			
Academic Institution:	University of Maryland, Baltimore County	**Major:**	Chemical Engineering
Academic Standing (Sept. '19):	Senior		
Future Plans (School/Career):	Work as a data analyst or programmer focusing in chemical engineering		
NIST Laboratory, Division, and Group:	MML, Materials Science and Engineering Division, Functional Polymers Group		
NIST Research Advisor:	Dr. Christopher Stafford		
Title of Talk:	Data Acquisition and Image Analysis of Small Angle Light Scattering		

Abstract:

This summer I created a program in MATLAB to automate image acquisition and analysis of surface wrinkling data. The goal of this program was to simplify the process of collecting and analyzing the gathered data with minimal work for the user. The new program is designed to interact directly with the camera for image acquisition, as well as analyze the images for intensity and/or peak position over time. Using the relative peak position or intensity over time, the wavelength or amplitude of the sinusoidal wrinkles can be calculated, respectively. This program can calibrate a given image with the camera to put peak positions in real space for later reference. Additionally, this program is capable of analyzing thousands of images in user specified regions of interest, generating graphs with requested data, and fitting data with proper parameters. The program also allows users to compare relative curves of different datasets. Finally, I created an algorithm to determine which images, and how many images, should be read as a function of time to speed up analysis and reduce noise in the data.

NCNR SURF Participants

First Name	Last Name
Emily	Blick
Hamna	Chaudhry
Candyce	Collins
Disha	Das
Marshall	Nakatani
Julianna	Price
Malgorzata	Psurek
Lizabeth	Quigley
Joseph	Rath
Spencer	Rodgers
Emma	Rogers
Andrew	Seamone
Racheal	Spruill
Washat	Ware
Mark	Zic

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Emily Blick			
Academic Institution:	The University of Maryland	**Major:**	Bioengineering
Academic Standing (Sept. '19):	Graduated		
Future Plans (School/Career):	Postbaccalaureate at The National Institute of Health		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron-Condensed Matter Science Group		
NIST Research Advisor:	Yun Liu		
Title of Talk:	Long-Term Vesicle Stability for Liposomal Nanomedicines		

Abstract:
Liposomes are promising candidates for future drug delivery applications due to the similarities in morphology to cellular membranes. The possibility of developing nanomedicines using phospholipid bilayer vesicles has sparked further investigation of pertinent liposomal properties. The understanding of vesicle stability is essential before they can be utilized in the pharmaceutical industry. Beginning last summer, my experiments have yielded interesting results showing that vesicle size, solution temperature, and oxygen exposure can have surprisingly large impacts on liposomal stability. In order to monitor vesicle properties dynamic light scattering (DLS) and small angle neutron scattering (SANS) techniques were used. DLS measured the apparent vesicle radius and was able to provide data on the change of vesicle size over time under varying conditions. On the other hand, SANS enabled us to see the change in physical structure of the liposomes over a wide range of length scales during the degradation of vesicles in solution. By combining these two techniques, observable changes in vesicle size, rigidity and structure were determined in relation to storage environment. The physical instability of the liposomes was linked to chemical degradation of the lipid molecules by either hydrolysis or oxidation. Each degradation method differs in both the pathways and final products that were distinguished through chemical assays. Our experimental results provide new insights on what conditions allow vesicles to remain stable and capable for future treatment use.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

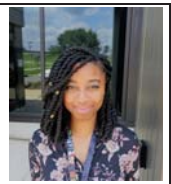
Name: Hamna Chaudhry			
Academic Institution:	University of Maryland University College	**Major:**	Computer Science
Academic Standing (Sept. '19):	Junior		
Future Plans (School/Career):	Graduate Studies in Computer Science		
NIST Laboratory, Division, and Group:	NIST Center of Neutron Research, Reactor Operations and Engineering Group		
NIST Research Advisor:	Dagistan Sahin		
Title of Talk:	NBSR Reactor Plant State Predictor		

Abstract:

National Institute of Standards of Technology (NIST) has a nuclear reactor (NBSR: National Bureau of Standards Reactor) which is currently undergoing console upgrades. The Operators need to be trained to become familiar with the NBSR console before implementing changes on the console. Use of Mixed Reality (MR) for strategy optimization and reactor operator training provides a modular and effective environment. However, the existing MR platform does not provide a realistic simulation environment. The operator interactions and/or perturbations should result in feedback that are like the real reactor operation. The goal of this project is to create The NBSR Reactor Plant State Predictor (PSP) by implementing the components and functionality of the physical console that would behave comparable to the NIST NBSR reactor. The NBSR PSP is composed of two main components. The first component analyzes moving average trends and compares them to historical data, and the second component predicts expected values of each variable of interest using a trained neural network.

The determination is to use real data from the reactor to teach a machine which would predict reactor states based on the user input. The hologram is a realistic reactor operation console which will be used to interact with the simulated console.

Trend analysis will be accomplished by keeping historical and current moving average values of variables in a database. Time dependent data will be processed through an Auto-Regressive Integrated Moving Average model to represent characteristics of current conditions. Results will aid in making changes on the console design or operating procedures. Furthermore, reactor operators would experience realistic plant feedback while practicing operational procedures in the MR environment. Overall, this project has the potential to be a useful and applicable tool for reactor operators and the reactor engineers in the future.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Candyce Collins		
Academic Institution: Fayetteville State University		**Major:** Chemistry - Materials Science
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Obtain a Masters and Ph.D. in Chemical Engineering or Materials Science	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron-Condensed Matter Science Group	
NIST Research Advisor:	Kathleen Weigandt, Avanish Bharati	
Title of Talk:	When Polymers Meet: Self-Assembled Amphiphilic Diblock Copolymers	

Abstract:
The development of homogeneous anisotropic particles is difficult, labor intensive, and has limited scale-up possibilities. We adopted crystallization-driven self-assembly (CDSA) approach for the diblock copolymers to develop these anisotropic particles with varying aspect ratio. We took advantage of the fact that the self-assembly of diblock copolymers in a selective solvent is determined by the packing parameter of the polymer blocks, as well as the quality of the solvent. We asked the question: Can the shape and size of the particles formed during the self-assembly of diblock copolymers be altered by the packing parameter of the diblocks as well as the solvent quality? To examine these phenomena, diblock copolymers of Polyethylene Oxide (PEO) and Poly L-lactic Acid (PLLA) were used. With the aim to develop model particles for research, there was an attempt to optimize the conditions at which we could obtain rod-like structures; especially due to the thermodynamically driven repulsion of the block copolymers to one another, which leads to different morphologies. The choice of temperature, solvent mixture type - Tetrahydrofuran/D_2O versus Acetone/D_2O - and solvent quality was determined by studying the solubility of individual polymers using Dynamic Light Scattering (DLS) and Small-Angle Neutron Scattering (SANS). For the crystallization of the short PLLA core surrounded by the long amorphous PEO corona to form rod-like particles for certain block ratios, a marginal solvent ratio for both of the diblocks was chosen. The generated polydisperse particles obtained from the polymers, referred to as preseeds, were subjected to probe sonication to form fairly monodisperse particles, called seeds. By optimizing the solvent ratio to be good for the PEO corona and marginal to bad for the PLLA core, the growth of the PLLA from the diblock solution onto its crystal growth front in the seeds was pursued. DLS and SANS revealed that the desired solvent ratio was attained at 10 wt% Acetone to 90 wt% D_2O with a temperature of 25°C. Depending on the diblock concentration, the process of CDSA is expected to result in monodispersed particles with controlled aspect ratios. In the future, the findings will provide a toolbox of particles with varying aspect ratio to answer the fundamental questions relevant to the flow behavior of soft materials under industrially relevant conditions using a slit capillary rheometer in combination with SANS.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Disha Das		
Academic Institution: Carnegie Mellon University		**Major:** Computer Science
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Work in industry as a software engineer	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Reactor Operations and Engineering Group	
NIST Research Advisor:	Dr. Dagistan Sahin	
Title of Talk:	Performing Human Factors Analysis on Nuclear Reactor Console with Mixed Reality	

Abstract:

The nuclear reactor control console at the National Institute of Standards and Technology Center for Neutron Research is undergoing several modifications. The purpose of this project is to build an environment to perform Human Factors Analysis (HFA) on the proposed console changes.
HFA helps design a product so that humans will be able to easily interact with it, accounting for both physical and psychological factors. HFA is especially important with regards to critical systems such as nuclear reactors because human error is cited as a major cause in many of the most severe nuclear related accidents. Errors in operation can have significant consequences. HFA aims to minimize the likelihood of these errors and makes recognizing and responding to problems easier and faster.
To conduct HFA, a Mixed Reality (MR) platform will be used to simulate the reactor console and its operations. MR was chosen because it is portable, extendible, and less expensive compared to physical models. Additionally, the MR platform allows HFA to be conducted throughout the design process while allowing modifications to the design. The program will train reactor operators on how to perform different operating procedures as well as respond to situations that are not easy to simulate on the physical console. While training the reactor operator, the MR platform will log and analyze timing and correctness data. Then engineers will be able to look at this data and evaluate and compare proposed changes.
Overall, this project will create an environment that can be utilized for reactor operator training and human factors analysis, allowing for optimization of the Human Machine Interface in the reactor control room. This optimized interface will allow the reactor operators to improve the speed and accuracy with which they perform procedures.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Marshall Nakatani		
Academic Institution:	The George Washington University	**Major:** Biology
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Graduate School/Biological Research	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron-Condensed Matter Science Group	
NIST Research Advisor:	Ryan Murphy	
Title of Talk:	Capillary µRheoSANS: Lipid Vesicle Nanostructure and Rheology at High Shear	

Abstract:
High shear flows occur readily in biological and industrial processes such as spraying, coating, lubrication, intravenous drug delivery, and capillary flow. Standard rotational rheometers are typically limited to measuring viscosities of complex fluids up to shear rates of 1000 s^-1. However, a recently developed Capillary µRheoSANS device combines a high-pressure capillary rheometer and small-angle neutron scattering (SANS) to simultaneously measure the rheology and nanostructure of complex fluids at shear rates up to 1,000,000 s^-1. Pharmaceutical applications utilize suspensions of lipid vesicles, particularly for intravenous drug delivery, which solubilize and transport therapeutics into the circulatory system. However, the structural integrity of lipid vesicle formulations in capillary flow environments and high shear rates is poorly understood. To investigate the stability and deformation of lipid vesicles, a model lipid system containing 100 nm vesicles of dimyristoylphosphatidylglycerol (DMPG) was measured with capillary µRheoSANS. The steady shear viscosities of different DMPG vesicle concentrations were measured in a standard cone and plate rheometer, and the shear-thinning behavior was compared to the Capillary µRheoSANS measurements at higher shear rates. SANS data helped to further examine the structural properties of the vesicles at rest and under flow. The extent of scattering anisotropy increased with shear rate, indicating some degree of alignment or deformation under flow. It was also discovered that the average vesicle diameter appeared to decrease after prolonged flow in the capillary device, although the mechanism of this size change remained unclear. This research begins to address important questions about the behavior of lipid vesicles in extreme flow environments, while also highlighting the capabilities of the µRheoSANS instrumentation at the NCNR. Ongoing instrument design involves implementing temperature control and a motorized slit aperture to measure the fluid structure parallel to the direction of flow. The ability to measure the rheology and nanostructure at extreme shear rates and varying temperatures will benefit future research and development of complex fluids for various applications.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Julianna Price		
Academic Institution: Wilson College		**Major:** Biochemistry and Molecular Bio.
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Attain my Ph. D. in Pharmacology	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor:	Amy Xu	
Title of Talk:	Oral Insulin Delivery via Microencapsulation	

Abstract:

Diabetes mellitus is an endocrine disease characterized by abnormally high blood glucose levels as a result of insufficient insulin production or improper cell glucose absorption. Currently, 422 million adults are living with diabetes worldwide. In order to treat diabetes, insulin is most often supplemented through subcutaneous injections. This is difficult for many people who have a fear of needles and can leave room for improper /misusage. This research investigates two different insulin encapsulation methods that may be utilized to create a more efficient, oral delivery system for insulin in hopes that patients do not need to utilize injections. The first encapsulation method uses zein protein nanoparticles as carriers for insulin, the insulin-loaded zein nanoparticles are then stabilized through interactions with alginate or pectin polysaccharide. In the second method, the insulin-loaded nanoparticles are prepared through layer-by-layered assembly of oppositely charged chitosan and alginate polysaccharides. To evaluate each preparation method, dynamic light scattering (DLS), small angle neutron scattering (SANS), scanning electron microscopy (SEM) and protein gel electrophoresis (SDS-PAGE) were used to gain information on the size, shape, and insulin encapsulation efficiency of the nanoparticles created. Finally, release experiments are done in simulated digestive fluids (intestinal and gastric). Information on the release and diffusion of insulin from nanoparticles over time provides more insights into the bioavailability of insulin-loaded nanoparticles.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Malgorzata Psurek		
Academic Institution: University of Maryland - College	**Major:** Chemistry	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Graduate school, followed by a career in some form of environmental chemistry.	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor:	Dr. Terrence Udovic	
Title of Talk:	Breaking up the crystal lattice to improve superionic conductivity	

Abstract:

In today's rechargeable batteries, the electrolyte is a flammable, lithium-based liquid. Since mining lithium is relatively expensive and environmentally detrimental and the liquid electrolyte can spill or catch on fire, there is a need to find an alternative. A promising solution to this problem can be found in the solid-electrolyte salt $Na[CB_{11}H_{12}]$, which can conduct charge through its Na^+ cations as a without needing to be liquid or aqueous. However, in order to achieve a useful level of conductivity, the salt must be in its disordered state, which occurs above 110 degrees Celsius. We have shown that by dissolving $Na[CB_{11}H_{12}]$ in water and allowing it to infiltrate into the pores of nanoporous silica, the disordered state can be maintained even at very low temperatures. We load a silica substrate, by adding to it a saturated solution of $Na[CB_{11}H_{12}]$, making sure there is even contact of all the solution to all of the silica, and subsequently drying at 200 degrees Celsius to remove all water. We have studied how this salt interacts with various types of silicas through differential scanning calorimetry, x-ray powder diffraction, quasielastic neutron scattering, neutron vibrational spectroscopy, and AC impedance measurements. We have varied the pore size and shape, as well as explored high-surface-area silicas. The goal of this project is to determine the best SiO_2 and loading procedure for maximizing the ionic conductivity for this hybrid superionic material at room temperature.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Lizabeth Quigley		
Academic Institution: University of Tennessee at Knoxville	**Major:** Mechanical Engineering	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Grad School	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor:	Alex Grutter	
Title of Talk:	Depth Dependence of Skyrmions in Thin Films	

Abstract:

Skyrmions are recently discovered chiral magnetic structures with interesting topological features which make them ideal for use in future data storage and logic devices. Skyrmions are uniquely stable because their magnetic moments wrap into a closed loop structure which cannot be created, destroyed, or distorted continuously to form any other structure than a skyrmion. This magnetic moment geometry makes the skyrmions robust against system defects and allows them to be easily moved by an applied electric current. Like modern magnetic memory, in future thin film skyrmion devices, the surface will be read for the absence or occurrence of skyrmions, encoding '1's' and '0's', respectively. Therefore, it is critical to know how the surface of the skyrmion differs from the bulk.

Here, we study a thin film super-lattice of gadolinium and iron (GdFe) which forms skyrmions at room temperature and zero magnetic field, as necessary for integration into next-generation electronic devices. Most investigations into skyrmions have focused on the bulk-average characteristics of the skyrmions, and lack the ability to resolve the different surface and 'bulk' structure. However, grazing incidence small angle neutron scattering (GISANS) is sensitive to both the bulk and the surface of the material, much like electronic devices, and can distinguish them. Unfortunately, GISANS results are difficult to interpret on their own, so we used polarized neutron and X-ray reflectometry to define the depth dependence of the film and its magnetism. We made a model using the reflectometry data and the object oriented micromagnetic framework to simulate the GISANS data. The model can be changed until the simulated and measured GISANS data match. Once a model is obtained that reproduces the measured GISANS pattern, we will be able to resolve the depth profile of the skyrmion and compare against traditional skyrmions. This will significantly aid the development of skyrmion spintronics and accelerate their implementation into future technology.

SURF Student Colloquium

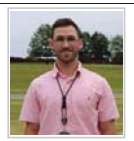
NIST – Gaithersburg, MD
August 5-9, 2019

Name: Joseph P Rath III		
Academic Institution: Rowan University	**Major:** Physics / Data Analytics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Graduate School (Condensed Matter Physics) / Full-Time Data Analyst	
NIST Laboratory, Division, and Group:	NCNR, Condensed Matter Physics	
NIST Research Advisor:	William Ratcliff, Paul Kienzle	
Title of Talk:	The Applications of Artificial Intelligence in Neutron Diffraction Analysis	

Abstract:

To understand the properties of a material, its structure must be determined at an atomic level. At NIST we do this by placing a material in a beam of neutrons, and by analyzing the consequent neutron diffraction, the crystal structure of said material can be revealed. Such analysis involves investigating the space around the material in search of neutron peaks, or specific angles at which the neutrons are being deflected into the detector by the structure of the material. This process is normally very time consuming because it involves human interaction and decision-making in deciding which angles should be explored. This is a problem because the number of neutron scattering facilities, such as NIST, is small and consequently makes time needed for measurement limited and very precious.

In an attempt to resolve this issue, we investigated whether a reinforcement learning algorithm could be used to increase the efficiency of instrument use. This is done by using the algorithm to learn if there are measurements that will provide us with more information than others, in determining crystal structure. Out of many different types of reinforcement learning algorithms, we chose the policy gradient approach (specifically, proximal policy optimization) due to the algorithm's efficiency in sampling large action spaces. Initial results using this algorithm yielded a promising output in learning about an example crystal structure, but further work will have to be done to perfect it.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Spencer Rodgers		
Academic Institution: West Virginia Wesleyan College	**Major:** Applied Physics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Physics or Engineering Grad School	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor:	Patrick Quarterman	
Title of Talk:	Probing Anomalous Field-Expulsion in Superconductor/Ferromagnetic Thin Films	

Abstract:

Recent experimental studies of superconductor/ferromagnet (S/F) bi-layers have observed anomalous field-expulsion that stems from electron interactions, when a superconductor is in contact with a ferromagnet. Electrons in a ferromagnet have their spins aligned, even in the absence of a field, resulting in a net magnetic moment. However, electrons in a superconductor form Cooper pairs, below the critical temperature, causing the material to have zero electrical resistance and expel external magnetic fields (i.e. Meissner effect) described by the London penetration equation. In a S/F heterostructure, Cooper pairs leak into the ferromagnet in a process known as the superconducting proximity effect. The recently theorized electromagnetic proximity effect occurs simultaneously with the superconducting proximity effect and has been proposed to explain the observed anomalous field-expulsion. This effect predicts that electrons from the ferromagnet leak into the superconductor, which creates a long-range magnetic field along the superconducting surface.

We search for these interactions using polarized neutron reflectometry (PNR) and x-ray reflectometry (XRR). PNR and XRR form a comprehensive picture of the nuclear and magnetic depth profiles of thin films. These depth profiles are the scattering length density (SLD) as a function of distance from the surface. We determine the nuclear and magnetic structure throughout the S/F bi-layers from interpretation of the SLD depth profile. By characterizing the magnetic field profile, we search for experimental evidence of the electromagnetic proximity effect on top of the Meissner effect. I will present our work to understand anomalous field-expulsion caused by interaction between superconducting and ferromagnetic thin films.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Emma Rogers		
Academic Institution:	Tulane University	**Major:** Biomedical Engineering
Academic Standing (Sept. '19):	Senior, B.S.E. Candidate	
Future Plans (School/Career):	Manufacturing engineer with biomedical electronics and microdevices	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron-Condensed Matter Science Group	
NIST Research Advisor:	Dr. David Hoogerheide	
Title of Talk:	The Development of Bilayer Overtone Analysis for Measuring Protein and Ion Activity	

Abstract:
The ability to maintain homeostasis between constantly fluctuating internal and external environments is essential for sustaining life across all living species. These life processes are mediated through the physical and organizational properties of the semipermeable lipid bilayer that forms the basic structure of the cell membrane. On a much smaller scale, the structure of the lipid bilayer governs the interaction of a wide range of membrane-associated proteins that are responsible for maintaining the gatekeeping function of the cell membrane from cell formation to cell death. However, the mechanisms by which many proteins associate with bilayer surfaces is insufficiently understood and such complex mechanisms are difficult to study with traditional solution-based biochemical methods. For these reasons, real-time measurements of protein interactions with lipid membranes are useful biophysical tools for characterizing particular classes of proteins that transiently associate and dissociate from the bilayer interface, like peripheral membrane proteins.

Bilayer overtone analysis (BOA) is a complementary technique that can be used to analyze the response of a lipid bilayer subjected to an alternating electrical signal. The lipid bilayer can be functionally modeled as a deformable capacitor with a transmembrane potential that changes in response to the binding of charged species, such as biological proteins or ions, to an exposed region of the bilayer surface. Changes in transmembrane potential can be measured to reveal the position, activity, and concentration of these membrane protein or ion interactions. A standard BOA setup consists of a physical cell in which two chambers are electrochemically isolated by a Teflon partition with a 100 μm diameter perforation to provide an interface for the formation of the free-standing lipid bilayer. This cell is then electrically stimulated by a lockin amplifier, which can be used to measure the transmembrane electrical response at the first and second harmonics of the excitation wave.

This project will establish a standard assembly of the BOA physical and electrical components, as well as the integration of the setup with updated control software and data collection platforms. It will then be shown that standard control measurements can be acquired for divalent ions, which will then be used to standardize the effect of small membrane-active phospholipases. These measurements will establish a quantitative basis for understanding the method by which membrane proteins and ions associate with lipid bilayers.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Andrew Seamone		
Academic Institution:	University of Colorado Boulder	**Major:** Civil Engineering
Academic Standing (Sept. '19):	1st Year Graduate Student	
Future Plans (School/Career):	Aerospace Engineering Graduate Student at University of Michigan, Ann Arbor	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Reactor Operations and Engineering Group	
NIST Research Advisor:	Danyal Turkoglu, Daniel Mattes	
Title of Talk:	Thermal-Hydraulics Feasibility for an Optimized Ultra-Compact Nuclear Reactor	

Abstract:

The current reactor at the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) has been operated since 1967 and is one of five high-performance research reactors in the United States. The reactor produces neutrons that are used in physics and materials science experiments. A replacement neutron source at the NCNR is desired because a disruption in neutron availability due to prolonged aging reactor maintenance or refurbishment would have a negative impact on neutron science within the United States and the scientific disciplines that NIST serves. A design study has identified an ultra-compact reactor core optimized for cold neutron science as a potential successor that would be world class as well as safe, reliable and cost-effective. With a high-power density, thermal-hydraulic considerations are crucial for safely removing 20 MW of fission power. Previous limitations in the design process came from using correlations to evaluate the thermal-hydraulics. I used a multi-physics solver, COMSOL, as part of an iterative design process that simulates the behavior of nuclear reactor core designs. Doing so produced studies of heat transfer, computational fluid dynamics, and fluid structure interaction which I evaluated to investigate best estimates for reactor core requirements rather than using conservative estimations. The use of correlations and COMSOL simulations provided insights on key geometric parameters for the core design that would keep safe margins from critical flow velocity and critical heat flux phenomena. As multi-physics simulations provide a reliable framework for evaluating and optimizing the reactor core, this project lays the groundwork for future COMSOL simulations as the design project progresses over the next several years.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Racheal Spruill		
Academic Institution: University of Maryland Baltimore County	**Major:** Biology, B.S., Sociology, B.A.	
Academic Standing (Sept. '19):	Senior (5th Year)	
Future Plans (School/Career):	Finishing my Master's and last year of undergrad, then pursuing an MD/Ph.D.	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group	
NIST Research Advisor:	Susana Teixeira	
Title of Talk:	SURFing with Green Tea: What Neutrons Read in Tea Leaves	

Abstract:

Green tea polyphenols contribute to its taste, aroma, and health benefits such as reduced risk of degenerative diseases and cancer. 85% of polyphenols in green tea are catechins, mostly Epigallocatechin gallate (EGCG), a potential alternative to synthetic food additives. EGCG has been shown to prevent the growth of bacteria responsible for food spoilage while showing antioxidant activity in food systems. Polyphenols are however susceptible to light, high extraction temperatures, and alkaline conditions, which cause their degradation during extraction and food processing. Several approaches have been used to improve polyphenol yields, stability, and production costs, including various solvent free extraction techniques, modification of the structure of EGCG or association with protein-based carriers. Bovine serum albumin (BSA), found in blood serum and milk, functions as a transporter of endogenous and exogenous compounds in the circulatory system and has been shown to bind and stabilize polyphenols. The nature of the interactions is thought to be mostly hydrophobic. The underlying mechanisms of BSA-polyphenol interactions, as well as their stability, are central to the development of effective carriers as delivery systems and to the engineering of improved food processing. While high-pressure (HP) is increasingly used in sterilization and food processing, HP is also a non-invasive tool for the study of protein-polyphenol interactions. This project combines neutron scattering and HP techniques to investigate the structure and stability of complexes of BSA with polyphenols, particularly EGCG. Small-angle neutron scattering (SANS) is a non-destructive technique that can be used to probe a broad range of interactions under various concentrations, temperature, pH and pressure conditions. The results highlight how neutron scattering can contribute new insights into polyphenol bioavailability in biological and food-processing environments.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Washat Roxanne Ware		
Academic Institution: Fayetteville State University	**Major:** Chemistry, Materials Science B.S.	
Academic Standing (Sept. '19):	Junior	
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. Antonio Faraone, Dr. Elizabeth Kelley	
Title of Talk:	Using Viscoelastic Properties of Polymer and Lipid to Study the Cell Membrane	

Abstract:
The lipid bilayer is one of the most important components of the cell membrane and plays a critical role providing a barrier between the cytoplasm inside of the cell and the outside of the cell. These membranes are also soft, and their structure and dynamics are affected by the elasticity of the cytoskeletal network and the extracellular matrix that surround the cell. Here we developed a model system to study how the properties of the surrounding matrix environment affects the lipid membrane dynamics. We used polyethylene glycol polymer solutions with well-defined viscoelastic properties to mimic the complexity of the cell environment. We characterized the properties of the polymer solutions with rheology, dynamic light scattering, and small angle neutron scattering. We then prepared liposome vesicles made from DMPC and DMPG in polyethylene glycol solutions of different concentrations and molecular weights. We measured the diffusion of the liposomes in the polymer solution and determined the rigidity and other mechanical properties of the liposome membrane as the viscosity of the surrounding medium is varied. We discovered that the viscosity of the polymer solution had significant impact on the dynamics of the liposome vesicles. Knowing how the properties of a lipid bilayer are affected by its surroundings can help researchers better understand the cell membrane dynamics and may one day help others in the medical field find more efficient ways to deliver drugs.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Mark Zic		
Academic Institution: University of Maryland, College Park	**Major:** Physics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Pursue a Ph.D. 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:	Neutron Scattering Study of a Triplet Superconductor	

Abstract:

In a superconductor, electrons with opposite spin typically pair in a singlet state. However, in the rare case that Cooper pairs are bound in the triplet state, ferromagnetic fluctuations have been proposed to make the superconductor unusually resistant to the usual detrimental effects of magnetic fields, leading to an extremely large value of the upper-critical field.

We recently discovered triplet superconductivity in the actinide superconductor UTe_2. Of the familiar triplet superconductors, URhGe and UCoGe, UTe_2 does not undergo a ferromagnetic phase transition. Instead, the paramagnetic state is expected to house ferromagnetic fluctuations. We probe these fluctuations in a manner similar to the critical fluctuations of conventional ferromagnets; we examine UTe_2 above a proposed transition at 0 K, also known as a quantum phase transition. This requires low temperatures (below 2 K) and high magnetic fields (up to 8 T) in order to induce a correlation above the transition temperature. Small angle neutron scattering (SANS), a technique used to observe magnetic correlations in materials by taking the Fourier transform of a magnetic signature in a real-space magnetic material, is ideal for probing long-range ferromagnetic correlations.

In this talk, I will present our work using SANS to study UTe_2.

PML

PML SURF Participants

First Name	Last Name
Arjun	Agarwal
Caroline	Azadze
Adam	Brewer
Julia	Codere
Michael	Doris
Jack	Fletcher
Mark-yves	Gaunin
Franklin Nicolas	Gavilanez Villalta
Kathryn	Gill
Liza	Gunther
Matthew	Ishimaru
Robert	Kauffman
Caitlin	Lee
Gillian	Lee
Thomas	Marsh
Elieser	Mejia
Amber	Meyers
Michelle	Morris
Peter	Orban
Jesus	Perez
Nikita	Podobedov
Guadalupe	Quirarte
Tojo	Rabemananjara
Heriniaina	Rakotomanana
Holland	Rhodd-Lee
Amberly	Ricks
Russell	Schwartz
Macrae	Smith
Hristiana	Stoynova
Benjamin	Wade
Hunter	Wages
Eli	Weissler

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Arjun Agarwal		
Academic Institution: University of Maryland	**Major:** Aerospace Engineering	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Attend graduate school researching space electric propulsion.	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Optical Technology Division, Group 684	
NIST Research Advisor:	Dr. Gillian Nave	
Title of Talk:	Vacuum Ultraviolet Fourier Transform Spectroscopy of Iron Group Elements	

Abstract:

Satellites such as the Hubble Space Telescope and the James Webb Space Telescope, rely on databases of accurate molecular and atomic spectroscopic data for interpreting astrophysical phenomena. NIST assists in this effort my maintaining the Atomic Spectroscopy Database (ASD). The information within ASD is produced using a variety of instruments, models, and analytical techniques. This variety provides data spanning the entire electromagnetic spectrum, which is required in order to holistically interpret astrophysical data.

This project focused on constructing a Fourier transform spectroscopy (FTS) setup that was able to cover the vacuum ultraviolet (VUV) region. VUV light is absorbed in air, requiring VUV Fourier transform spectroscopy to be done under high vacuum. The interpretation of astrophysical data using molecular and atomic spectroscopic data also requires highly accurate measurements, resulting in a FTS that must be able to provide data with very low uncertainties.

By completing the FTS setup, we were able to begin measuring the relative intensities of spectral lines in iron group element spectra for astrophysically relevant reference data such as branching fractions.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Caroline Azadze		
Academic Institution: Cornell University	**Major:** Electrical and Computer Eng.	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Graduate school	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Applied Electrica	
NIST Research Advisor:	Gerald FitzPatrick, Kang Lee, Eugene Song	
Title of Talk:	Performance Measurements of Smart Sensor in Smart Grid	

Abstract:

A smart grid is an electrical grid which includes an integration of a variety of operation, technologies and energy measures including smart sensors, smart meters, smart appliances, renewable energy resources, and energy efficient resources. Electronic power conditioning and control of the production and distribution of electricity are important aspects of the smart grid. Consequently, engineers regularly need to test and calibrate power quality devices such as smart sensors to ensure that input and output voltages and currents are within certain required accuracy and dynamic ranges to function with other devices properly as a system. Often, smart sensors and measurement systems are used to support standard production and distribution of electricity as intended for this project.

Our research is mainly focused on developing National Instruments (NI) LabVIEW Software to enable the integration of multi-channels NI PXI 5922 precision scope modules for the measurement of three-phase currents and voltages from a high precision power source. The results will be compared with measurements of the distorted currents and voltages measured by commercial merging units (MUs). These MUs, considered as smart sensors, acquire analog AC currents and voltages from conventional current and voltage transformers installed in the electric grid, convert them to the digital domain and transmits them in a form of sampled values (SV) through an Ethernet LAN to monitoring and protection devices.

For the comparison and analysis of our data samples, we developed a MATLAB model to perform Fast Fourier Transforms (FFT) and measurement uncertainty analysis of the sampled data collected from the NI scopes and the MUs. We used timing synchronization devices to enable real-time data sampling for accurate and precise comparison. In addition, we intend to test the entire system with a standardized harmonic signal in order to study the capability of the MU working with AC signals of various harmonics content.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Adam Brewer		
Academic Institution: The George Washington University	**Major:** Computer Engineering	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	I plan to have a career in Computer Engineering	
NIST Laboratory, Division, and Group:	PML, Nanoscale Device Characterization, Alternative Computing	
NIST Research Advisor:	Mark Stiles	
Title of Talk:	Programming Automated Programming	

Abstract:

The Alternative Computing Division at NIST deals with micro scale computing components that use novel technologies such as Memristors and Magnetic Tunneling Junctions. When designing chips that test these novel technologies, the researchers often use a Program called Cadence Virtuoso. The designs that they make often have over 400 pads, which are what allow the world inside the chip interact with the world outside of it. These pads are put into a frame that can be quite troubling to put together manually and this could take multiple days to do correctly. This made it a necessity to have a program which could take in what the researchers want the pad frame to look like and output that out nearly immediately. The program to do this was mainly made in Python and is a program that automates programming. The python code is used essentially to write SKILL code for the user. SKILL is a programming language based on LISP which Virtuoso uses. The user inputs what they want and the python code interprets that using a list. Then, iterating through this list, the program can see which pads need to go where. Based on what the list says, it sends the correct SKILL line into a file in which Virtuoso can read. The program is also being made to automate the placement of a power distribution grid onto the chip. This program will decrease the amount of time researchers here at NIST as well as at GWU and UMD have to spend making pad frames which will increase the amount of time they can spend doing the actual research.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Julia Codere		
Academic Institution: University of Maryland	**Major:** Physics	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	I plan to pursue a graduate degree in physics.	
NIST Laboratory, Division, and Group:	Physical Measurements Laboratory, Quantum Measurements Division, Applied Electr	
NIST Research Advisor:	Richard Steiner	
Title of Talk:	Analysis of the Harmonics of Distorted Power Waves from Smart Watt-hour Meters	

Abstract:

Smart watt-hour meters are used by utility companies to read electrical power so that customers are charged according to their energy usage. These meters are digital, unlike the analog mechanical meters that were used in the past. The smart meters may be inaccurate when reading the voltage and current from nonlinear loads, such as electronics and LED lights. A testbed of different loads was previously created to allow for an examination of the accuracy of the meters. During this project, we tested eight meters by comparing the power they measured to the power measured by a calibrated power meter.

Dimmable and non-dimmable LED light bulbs and dimmers were used to create a variety of current waveforms that were not like the sinusoidal waveforms that linear loads, such as incandescent bulbs, produce. The waves generated by the LED bulbs were distorted. How spiky a wave is can be measured by using the crest factor, a ratio of the peak to the root-mean-squared value. Simulations of different waveforms were made in Python to reproduce the data and analyze the crest factor in a more systematic manner. We are developing a way to improve the analysis of the accuracy of the meters by using a program created in LabVIEW to extract the harmonics of the current waveform. The harmonics are a breakdown of the wave and may be a better representation of the wave distortion than the crest factor. This will improve future analysis of measurements taken with different combinations of loads.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Michael Doris		
Academic Institution: California State University, Chico	**Major:** Physics & Electrical Engineering	
Academic Standing (Sept. '19):	Graduate	
Future Plans (School/Career):	Graduate School, PhD in Physics	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Radiation Physics Division, Neutron Physics	
NIST Research Advisor:	Dr. Michael G. Huber	
Title of Talk:	Eliminating Thermal Gradients For Neutron Interferometry	

Abstract:

Neutron interferometry is a powerful and sensitive tool used to explore quantum mechanics, test fundamental laws of physics, and measure important physical constants. Constructed from a single piece of perfect silicon, neutron interferometers manipulate the neutron wave-function to measure the quantum phase difference between two neutron paths. Their measurement sensitivity comes with the downside of a systematic coupling to environmental factors such as vibration and heat. To combat measurement noise from the environment, the Neutron Interferometer and Optics Facility (NIOF) at the NIST Center for Neutron Research (NCNR) was built to isolate the interferometer from external acoustics, seismic vibrations, and temperature variations. Although this facility offered superior isolation and stability, small thermal gradients across the crystal interferometer have persisted. These thermal gradients are now the leading systematic in neutron interferometric measurements. In response to this issue, additional passive and active temperature control mechanisms have been added to the NIOF. Following the "Box within a Box" approach, the interferometer is placed within an insulated enclosure equipped with Proportional, Integral, Derivative (PID) controlled heating systems. This talk will detail the results of using a modified approach to PID control in an attempt to reduce thermal gradients across the interferometer and improve the reliability and accuracy of neutron phase measurements.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Jack Fletcher		
Academic Institution: Missouri University of Science and Tech.	**Major:** Nuclear Engineering	
Academic Standing (Sept. '19):	Sophomore	
Future Plans (School/Career):	Ph.D./Research at national laboratory	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Division 685, Group 01	
NIST Research Advisor:	Stephen Eckel	
Title of Talk:	Lithium-7 Gray Molasses	

Abstract:

An absolute sensor of vacuum is needed for the ultra-high vacuum to extreme-high vacuum regime. The proposed cold-atom vacuum standard relates the lifetime of laser-cooled lithium "sensor" atoms confined in a magnetic trap to the frequency of their collisions with ambient gas in the vacuum, subsequently providing an absolute measurement of the pressure in the chamber.

Laser cooling of lithium below its Doppler limit (140 μK) is necessary to load the magnetic trap, but complicated by unresolved excited-state hyperfine structure on the D2 optical transition used for laser cooling. One approach to realizing sub-Doppler temperatures is gray optical molasses. Its application on the D1 transition permits the use of velocity-selective coherent population trapping, wherein atoms with nonzero momentum experience restoring forces from six counterpropagating beams, slowing the atoms into a "dark," non-absorbing state. In our experiment, a sample is first confined and cooled in a magneto-optical trap (MOT) operating on the D2 transition, then the gray molasses is performed on the D1 transition.

Gray molasses cooling is anticipated to decrease the temperature of lithium samples in a MOT below the Doppler limit to temperatures on the order of 10^-5 K. Ultimately, such a sample may be selected to serve as a primary standard of vacuum in the regime of 10^-6 to 10^-10 Pa with minimized uncertainty.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Mark-yves Gaunin

Academic Institution: San Diego State University | **Major:** Computer Engineering and Physics

Academic Standing (Sept. '19):	Undergraduate Junior
Future Plans (School/Career):	PhD in quantum information systems/quantum device characterization
NIST Laboratory, Division, and Group:	PML, Nanoscale Device Characterization Division, Atom Scale Device Group
NIST Research Advisor:	Garnett Bryant
Title of Talk:	Atomic-Scale Quantum Plasmonics

Abstract:

Classically, a plasmon can be described as an oscillation of electrons in a metal. Plasmons play a large role in properties of metals and semiconductors. Recently, the need to study the quantum characteristics of plasmons has arose due to the decreasing size of plasmonic nanoparticles: the Atomic Scale Device Group at NIST is able to place individual dopant atoms in a semiconductor with atomic precision in order to make a variety of quantum structures. Since a theory for quantum plasmons in nanoparticles is a large task to undertake, we focus on atomic-scale solid state systems such as gold atoms on a surface or carbon nanotubes. To study plasmonic excitations in the quantum limit, we model atomic chains which allows us to breakdown the independent boson description of plasmons. We are able to calculate the many-body spectra of finite, short atomic chains in order to identify plasmonic excitations of these atomic-scale systems. Plasmons are the low energy excitations of the chain when electron-electron interaction is weaker than the single-particle hopping energy.

In a previous project, plasmonic properties of a simple atomic chain was studied. We expanded the project by including disorder, or imperfections found in all realistic quantum many-body systems. Disorder was modeled by a random distortion on the particle hopping and/or Coulomb interactions of the system. The system was modeled in a variety of combinations of weak/strong disorder affecting either hopping, Coulomb interactions, or both simultaneously for many random seeds. This produced variances in the energy excitations of the system and indentified the limit of plasmonic behavior.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Franklin Gavilanez

Academic Institution: University of Maryland, College Park | **Major:** Mechanical Engineering

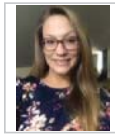
Academic Standing (Sept. '19):	Senior
Future Plans (School/Career):	Completing undergraduate degree and pursuing a career in product development
NIST Laboratory, Division, and Group:	PML, Sensor Science Division, Surface and Interface Metrology Group
NIST Research Advisor:	Alan Zheng
Title of Talk:	Intercomparison Study of Optical Measurement Methods for Toolmark Analysis

Abstract:

Spent cartridge cases and their connection to a specific firearm are an important aspect of forensic science and crime scene evidence. Upon ejection of a spent cartridge casing from a firearm, the cartridge casing is impressed with various characteristic markings, known as toolmarks.

There are currently various 3D topography measurement methods, such as disc scanning confocal, focus variation, photometric stereo, and programmable array continuous confocal microscope. The use of different methods can introduce variation in the measured surface of a spent cartridge casing. This project will focus on an intercomparison between the Alicona Infinite Focus, Nanofocus, and Evo Finder metrology instruments, which use focus variation, disk scanning confocal, and photometric stereo respectively.

To conduct the intercomparison study, the statistical differences of the surfaces must be measured and compared. To accomplish this, the Congruent Matching Cell (CMC) method, Aerial Cross Correlation function (ACCF), and Signature Difference (Ds) parameters will be used. The CMC method breaks up a reference topography into discrete cells and counts the number of congruent cells on the comparison topography, according to specified thresholds. A higher amount of congruent cells will correspond to a higher similarity. ACCF is a sililarity comparison of the entire area of each topography such that if they are identical, ACCF will be 100%. Ds is defined by the two topographies subtracted from eachother such that if they are identical, Ds will equal zero. Using these three parameters, the similarity of the different measurement methods can be quantified.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Kathryn Gill		
Academic Institution: East Carolina University	**Major:** Bio-Process Engineering	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Pursue a degree in biopharmaceuticals	
NIST Laboratory, Division, and Group:	PML, Sensor Science Division, Thermodynamic Metrology	
NIST Research Advisor:	Zeeshan Ahmed	
Title of Talk:	Photonic Biochemical Sensors and their use	

Abstract:

Environmental changes (global and local) greatly affects many important processes ranging from chemical synthesis, biological/pathological events, manufacturing and communication. Several sensing methods (e.g. electrochemical) have been developed and deployed to measure and monitor such changes in pursuit of greater sensitivity, accuracy, and precision. The National Institute of Standards and Technology (NIST) has been working with photonic-based sensors for parameters such as temperature, humidity, radiation hardness, and transient pressure. More recently, we have been in collaboration with NIST colleagues to explore the utility of photonic sensors in pH measurements. Unlike traditional electrochemical sensors, photonic sensors use properties of light, to make precise measurements. The sensor employs a commercially available photonic sensor known as a fiber-Bragg grating (FBG). The current work done has evaluated the photothermal response of a pH responsive hydrogel using an embedded temperature sensor (FBG). Specifically, the measurements conducted in this experiment use the photonic sensor to detect changes in the pH of a hydrogel- a polyethylene glycol (PEG) mixed with a photo initiator, hydrated in cabbage juice- at different wavelengths. The intent of these measurements is to identify and select the most appropriate process conditions, indicators, and sensor design to measure specific species of interest with hopes to create one photonic sensor that can measure multiple biochemical species simultaneously.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Liza Gunther		
Academic Institution: University of Maryland, College Park	**Major:** Physics	
Academic Standing (Sept. '19):	Sophmore	
Future Plans (School/Career):	Graduate school	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Nanoscale Device Characterization Division, Atom	
NIST Research Advisor:	Richard Silver	
Title of Talk:	Atom-Based Silicon Quantum Electronics	

Abstract:

Atom-based Si:P devices are a promising medium for developing the foundational bases of quantum computation: single electron and single atom transistors, and ultimately solid-state qubits. Using advanced hydrogen lithography and low-temperature epitaxial overgrowth, individual dopant atoms can be placed deterministically within a silicon lattice. Scanning Tunneling Microscope lithography enables the fabrication of donor-based qubits as well as the construction of atomically precise artificial molecules and 2-D superlattices in silicon. A primary objective is therefore to use this technique to demonstrate a functional multi-qubit architecture to produce scalable solid-state quantum computing. Typical devices consist of a source, drain, single-electron transistor (SET), and multiple gates and donor dots. Voltages are applied to the gates and the source/drain to control tunneling of electrons through the device. When there is enough electric potential, an electron will tunnel between the source/drain and SET, or between the SET and donor dots. In the presence of a magnetic field, the applied voltages are used to control the spin (and presence) of single electrons on the donors, while the SET can be used to remotely monitor the quantum state of the donors. With a time-varying magnetic field, the quantum states of the system can be manipulated to produce qubit operations for quantum computation.

Capacitance modeling is used to predict device electrostatics at the atomic scale. Computer-aided design and FastCap calculations are used to determine what precise device geometry will yield the desired electrostatic functionality. The present goal is to control capacitive coupling between device components so that the relevant energy scales for qubit operation are accessible. Once the devices have been produced, Atomic Force Microscopy and Peak Force Kelvin Microscopy are used to evaluate and locate the buried atomic structures in silicon. Capacitance modeling and microscopy are to be used in developing, testing, and characterizing the devices.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Matthew Ishimaru		
Academic Institution: Brown University	**Major:** Physics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Pursue a PhD in physics, become an astronaut.	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory,	
NIST Research Advisor:	Sujitra Pookpanratana	
Title of Talk:	Stable Foundations for Quantum Computing: Characterizing van der Waals Materials	

Abstract:

Quantum computation is an emerging field that involves manipulating quantum effects to perform calculations. It has the potential to hugely outperform classical computers in several areas including breaking many modern forms of encryption. A quantum bit based on topological quantum computing could allow for more stability than current technologies by using a class of materials known as topological insulators, which have an insulating interior but a conductive surface. This project investigates one of these materials: bismuth selenide (Bi2Se3).

Bi2Se3 is a van der Waals material, meaning that it is made up of repeating units of bonded layers connected to each other by weak van der Waals forces. This structure allows the surface of van der Waals materials to be cleaved off into two-dimensional structures through a process known as exfoliation. Because the electronic properties of Bi2Se3 are surface-sensitive, it is imperative that the surface be clean and uniform. This project developed a technique for using exfoliation to create Bi2Se3 surfaces suitable for analysis.

We focused on two van der Waals materials in this project: Bi2Se3 and highly ordered pyrolytic graphite (HOPG). HOPG is the bulk form of graphene, a well-studied two-dimensional material, and is readily available. We used HOPG to refine our exfoliation and measurement techniques.

Samples of HOPG and Bi2Se3 were prepared using manual exfoliation. The exfoliated layer and the newly exposed surface were both analyzed using X-ray photoemission spectroscopy (XPS), Raman spectroscopy, and atomic force microscopy (AFM). These techniques allowed us to measure the elemental and molecular composition of our samples, as well as their morphology. Through this analysis, we were able to confirm that our exfoliation produced a clean and uniform surface suitable for further study.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Robert Kauffman		
Academic Institution: Juniata College	**Major:** Physics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Graduate School	
NIST Laboratory, Division, and Group:	PML, Quantum Measurement, Laser Cooling and Trapping	
NIST Research Advisor:	Ian Spielman	
Title of Talk:	Automated Fiber Coupling with Machine Learning Optimization	

Abstract:

Machine learning is the scientific study of algorithms and statistical models that computer systems use to perform specific tasks without explicit instructions. One essential aspect of machine learning algorithms is optimization. Elementary optimization routines such as gradient descent and downhill simplex are used to minimize or maximize the cost function of a task. In the laser cooling and trapping laboratory, optimization algorithms are used in many aspects of experimentation to increase the number of cooled atoms and decrease the overall experimentation time. For this project, machine learning optimization is used to automate the pre-experimentation task of coupling a laser into a single mode fiber. Using New Focus PICOMOTORs and python, the process of fiber coupling two mirrors with four degrees of freedom is done automatically using a computer program. The goal of the project is to both maximize the amount of power coupled into the fiber and create a quicker and more efficient coupling process. This talk will explain the basics of machine learning optimization and its importance in research laboratories, as well as investigate the effectiveness of the created fiber coupling algorithm and its efficiency versus coupling by a skilled human hand.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Caitlin Lee		
Academic Institution:	University of Maryland, College Park	**Major:**	Electrical Engineering
Academic Standing (Sept. '19):	Sophomore		
Future Plans (School/Career):	Obtain undergraduate degree, possibly attend graduate school		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Fundamental Electrical Measurements Group		
NIST Research Advisor:	Dean Jarrett		
Title of Talk:	Improvements to the Dual Source Bridge System for Calibration of High Resistance Standards		

Abstract:

The Metrology of the Ohm project is responsible for calibrating and maintaining resistance standards. Accurate calibration of high resistance standards requires the use of transfer standards, dual-source bridges, and precise low current measurements. The basis of this project is to begin the process of implementing updates to the present dual-source bridge system. One such update involves the possible replacement of the sources within the bridge. The linearity of a source is one indication of the source's reliability; hence, linearity must be determined prior to implementation. This was accomplished by using an 8.5-digit digital multimeter to measure the voltage output, then comparing the measured output to the source's nominal output at various voltages within each voltage range. The dual-source bridge system implements a voltage ramping algorithm, in which the outputs of the sources are gradually increased or decreased to the desired final voltages. The effect of voltage ramping on the settling time of the current was observed by measuring the null current through the bridge. Measurements were taken for both voltage polarities, as well as with and without ramping. In addition, the effects of various cable types on settling time were observed. LabVIEW applications were created to automate all data collection processes. The results of these experiments will indicate any abnormal or unexpected behavior, so that changes to the hardware and/or software of the bridge can be made. The main update to the calibration system involves the translation of the application software. The calibration algorithm, which includes instrument controls as well as calculations and collection of data, is currently written in VisualBasic, an outdated programming language that may no longer be supported or available on laboratory computers, thus motivating the transfer of the program into LabVIEW.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name:	Gillian Lee		
Academic Institution:	University of Maryland, College Park	**Major:**	Electrical Engineering
Academic Standing (Sept. '19):	Sophomore		
Future Plans (School/Career):	Complete undergraduate degree, considering graduate school		
NIST Laboratory, Division, and Group:	PML, Microsystems and Nanotechnology Division, Biomedical Microtechnologies Group		
NIST Research Advisor:	Veronika Szalai		
Title of Talk:	Using Potentiometry to Determine Spin Concentration for Electron Paramagnetic Resonance (EPR) Spe		

Abstract:

Electron paramagnetic resonance (EPR) spectroscopy is used to detect and study paramagnetic samples via the magnetic properties of their unpaired electrons. The spin of an unpaired electron causes it to behave as a magnetic dipole. Applying a static magnetic field to a paramagnetic material causes the energy levels of the unpaired electrons to undergo Zeeman splitting. When the energy of a microwave quantum is equivalent to the energy level separation, the sample absorbs the microwaves, leading to an EPR signal. The integrated intensity of this signal is proportional to the amount and concentration of the sample. Thus, the concentration of spins in a paramagnetic sample can be quantified by comparison against a material of known volume and concentration.

The aim of the project is to develop a protocol for precise quantification of the amount of paramagnetic material within a given material. The free radicals α,γ-Bisdiphenylene-β-phenylallyl (BDPA) and (2,2,6,6-Tetramethylpiperidin-1-yl)oxyl (TEMPO) are stable at room temperature, and thus are widely used to determine spin concentrations in EPR spectroscopy. Most researchers assume a one-to-one correspondence between mass of these materials and number of spins, an assumption that is not accurate. Because free radicals display redox behavior, potentiometric titration is a possible method to determine the number of stable free radicals within a measured quantity of a given sample. Based on the reported reduction potentials of BDPA and TEMPO, tetrakis(dimethylamino)ethylene (TDAE) was chosen as a reducing agent. To the best of our knowledge, this is the first attempt to develop a potentiometric titration protocol for determining the spin concentration of an unknown sample of a stable free radical.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Thomas Marsh		
Academic Institution: Hamilton College	**Major:** Physics / Computer Science	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Attending graduate school to pursue a PhD in Physics	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Division 682, Neutron Physics Group	
NIST Research Advisor:	Daniel Hussey	
Title of Talk:	Analyzing spot weld strain using Neutron Bragg Edge Tomography	

Abstract:

Neutron imaging is an important tool for probing the bulk structure and properties of materials for a wide array of research areas. Since neutrons interact with material primarily through the strong nuclear force, many metals that can be difficult to study using traditional methods — such as X-ray imaging — are able to be analyzed using neutron imaging. Neutron tomography is a form of neutron imaging where images are taken at hundreds of individual angles as a sample is rotated and then are reconstructed using a filtered back projection algorithm to create a three-dimensional image of the sample's neutron attenuation coefficient in three dimensions.

We seek to use neutron tomography to attempt to quantify the strain caused by individual spot welds made with laser pulses of varying power levels on stainless steel disks. By gathering neutron tomograms over a range of wavelengths, we are able to utilize the change in neutron attenuation due to Bragg scattering to locate the "Bragg Edge" at each point in the sample which allows us to map deformations in the crystal lattice. Our method allows for an estimate of the strain in the sample along the beam direction to be made in less time and with a higher spatial resolution than more traditional methods of strain measurement.

The strains caused by a laser weld are of particular importance to metal additive manufacturing, where laser welds are used to entirely fabricate metal components. Thus, an increased understanding of the strain in individual spot welds could give an increased knowledge of the mechanical properties of additively manufactured components.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Elieser Mejia		
Academic Institution: Virginia Tech	**Major:** Electrical Engineering	
Academic Standing (Sept. '19):	First Year Masters Student at Virginia Tech	
Future Plans (School/Career):	Ph.D in Materials Science & Engineering/Researcher at a National Lab	
NIST Laboratory, Division, and Group:	PML, Microsystems and Nanotechnology, Photonics and Plasmonics	
NIST Research Advisor:	Amit Agrawal	
Title of Talk:	Nanoscale Engineering of Optical Resonances using Metasurfaces	

Abstract:

In recent years, a plethora of applications have become possible within modern photonics as a result of an enhanced understanding of light-matter interactions at the nanoscale. This has further allowed for precise tuning of optically induced responses using nanoscale fundamental building blocks constituting nanophotonic devices. Herein, the focus is on those applications which take advantage of optically resonant metallic and all-dielectric subwavelength nanostructures to include biosensing, lasing, active photonics, and nonlinear optics. The confinement of light and its ability to yield electric and magnetic resonances within metal-dielectric-metal and all-dielectric building blocks is explored through numerical simulations in which the former is tailored for high absorption. An emphasis is placed on the fabrication procedure which entails the use of phase shifting lithography,, e-beam evaporation, electron beam lithography, and reactive ion etching. Methods such as scanning electron microscopy and dark/bright field spectroscopy are utilized to characterize respectively the structure and optical response of these devices. Lastly, the acquired results are correlated with the potential applications for each device, i.e., highly absorptive optical nanoantennas for neural stimulation and recording, as well as high-Q all-dielectric metasurfaces exploiting the physics of bound states in the continuum to enhance nonlinear parametric processes such as higher harmonic generation.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Amber Meyers

Academic Institution: Hood College | **Major:** Chemistry

Academic Standing (Sept. '19): Senior

Future Plans (School/Career): Career in the industry, maybe graduate school

NIST Laboratory, Division, and Group: PML, Nanoscale Device Characterization, Nanoscale Spectroscopy

NIST Research Advisor: Dr. Ted Heilweil

Title of Talk: Ultrafast laser spectroscopy to study photodynamics of asymmetric hydrogenases

Abstract:

In nature, some bacteria are able to efficiently produce hydrogen gas. [FeFe]-hydrogenases are the enzymes that catalyze the production of hydrogen in nature. These enzymes, which contain iron in their active site, are of great interest because of the increasing need to develop a cheaper substitute for platinum as a catalyst for hydrogen production. Symmetric model compounds containing all CO ligands or mixed CO/CN and CO/PMe3 ligands on both irons in the active site have been studied extensively. However, this work will examine asymmetric molecules containing mixed CO/CN ligands: [Fe2(μ-S2C2H4)(CO)5(CN)1]1− (1) and [Fe2(μ-S2C3H6)(CO)5(CN)1]1− (2). The asymmetry of these model compounds makes the redox potentials of the two iron atoms different, therefore changing the compounds catalytic properties. The molecules are being studied using 400 nm and 266 nm UV pump pulse-infrared probe spectroscopy in order to better understand how the hydrogenase's active site interacts with light.

So far, we have studied 1 using a 400 nm pump pulse and observed distinct bleaches around 1930, 1979, 1999, and 2038 cm-1. We also saw new absorptions at 1899, 1964, and 2023 cm-1. The bleaches and absorptions decayed with a time constant of 23 +/- 6.6 ps. There is some evidence of residual signal remaining out to 300 ps, especially with the bleach at 1979 cm-1. We also tried pumping with 266 nm light but were unable to identify any signals, so far.

Studies on 2 using a 400 nm pump pulse are currently underway. Initial results show similar behavior to 1.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Michelle Morris

Academic Institution: Virginia Tech | **Major:** Biomedical Engineering

Academic Standing (Sept. '19): Sophomore

Future Plans (School/Career): Graduate with a Bachelor's Degree in Biomedical Engineering

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Microsystems and Nanotechnology Division, Biology Group

NIST Research Advisor: Dr. Arvind Balijepalli

Title of Talk: Field Effect Transistors Offer a New Level of Sensitivity for Biological Measurements

Abstract:

Field-effect transistors (FETs) have been the building blocks of microprocessors for decades. However, they have proven to be more versatile than their conventional application in computers. Due to their ability to amplify small signals, they have the potential to serve as precise sensors for a large variety of biological measurements. Since a majority of these biomolecular interactions are electrostatic, they can be directly detected by the charge-sensitive FETs, allowing for label-free analysis that is quicker and safer than previous forms of biological measurements that rely on radioactive or fluorescent labeling. With precision medicine being at the forefront of healthcare research, the capacity to detect specific biological activity at physiological levels is an important advantage that can lead to an earlier diagnosis, and therefore a more effective treatment of diseases.

This summer, I characterized dual-gated FETs for use in biosensing measurements. The dual-gated design of the FETs allowed for a small charge applied to the top gate to be amplified by the back gate. I tested two different dual-gated FET devices: solid-state FETs and liquid-gated FETs. Both designs allowed for back-gate amplification of a signal applied to the top gate. However, the solid-state device's top gate dielectric was formed by a metal oxide, while the liquid-gated device used an atomically-thin ionic liquid, allowing for higher sensitivity than that of the solid-state device. For the FETs to be reused, we conducted our biological experiments on an extension of the top gate. This allowed a separation of the biological components from the top gate dielectric. In this configuration, we were able to record pH values with a sensitivity of over seven times the Nernst value (~59 mV/pH). The low noise of the recordings also allowed a pH resolution within 0.0164 of the actual value with 95% certainty.

One of the key benefits of electronic measurements is their portability. Working towards the use of the dual-gated FETs in clinical settings, we developed a portable FET-computer interface by using a Raspberry Pi. As a first step to developing this interface, we used an analog voltage output "hardware-on-top" (HAT) attached to the Raspberry Pi to apply a voltage to a FET and record its current. This interface will be employed to measure the activity of neuronal cells and is currently being further developed.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Peter Orban		
Academic Institution: St. Mary's College of Maryland	**Major:** Mathematics and Physics	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Attend a PhD program for Applied Physics	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science Division, Fluid Metrology Group	
NIST Research Advisor:	Dr. Iosif Shinder and Dr. Aaron Johnson	
Title of Talk:	Improving Stack Flow Measurements by Making Them Faster and More Accurate	

Abstract:

Accurate flow measurements are essential for measuring the amount of pollutants emitted by industrial smokestacks. Stack flows have complex (i.e., skewed, swirling) velocity fields that degrade the performance of stack flow meters. Federal regulations require that stack flow monitors are calibrated at least annually. Calibrations are performed by averaging velocity measurements made at discrete points in the stack cross section. Today, most of these measurements are made using a two-dimensional probe called an S-type pitot probe, which only measures two components of velocity. In cases where the stack flow is three-dimensional, the S-type pitot probe can have significant errors. Although three-dimensional pitot probes such as the five-hole spherical probe have been developed to measure the entire velocity vector, this probe is time intensive to use since it must be nulled before each velocity measurement. The nulling process involves rotating the probe about its axis until the differential pressure between two ports on the probe equals zero. Factors such as swirling flow and turbulence also make this process extremely difficult and inaccurate.

To reduce measurement time and improve accuracy, we developed a non-nulling method to eliminate the need to rotate the probe. The NIST Wind Tunnel was used to calibrate pitot probes for which the non-nulling method can be used. Calibration factors are calculated from the differential pressure measurements. The calibration curves are currently fit with brute force: multivariable polynomial functions, often containing hundreds of parameters. In this work we implement a theoretical model based on potential flow to provide a physical basis for the curve fit. These curves can now be successfully fit with as few as three additional empirical parameters. Analytical solutions for the non-nulling procedure have been calculated under specific conditions, yet more work must be done to develop a generalized analytical solution.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Jesus Alberto Perez		
Academic Institution: University of California, Los Angeles	**Major:** Physics	
Academic Standing (Sept. '19):	Incoming graduate studetnt for fall 2019	
Future Plans (School/Career):	Professor	
NIST Laboratory, Division, and Group:	PML	
NIST Research Advisor:	Joseph Kopanski	
Title of Talk:	COMSOL Simulations of Electromagnetic Test Structures	

Abstract:

The demand for high performance computing has resulted in the vertical stacking of chips to maximize speed while minimizing power consumption. In such a configuration, the reliability of the entire stack depends on the integrity of the materials used, such as the metal interconnects. As these materials age their electrical and thermal properties shift and the performance of the devices drift from the values used in the original design.

Through the use of microwaves (1-20GHz), we are able to probe the physical state of the interconnects in prototypical 3D-ICs after thermal cycling. Specifically, we utilize the scattering parameters to acquire the electrical properties (i.e., resistance, inductance, conductivity, and capacitance (RLGC)) of strip lines. In order to fully understand the observed changes in the electrical properties with age, we need to explore the physics of failure of these materials. We have attempted to accomplish this by simulating the material changes with COMOSOL Multiphysics. A side-by-side comparison of the experiment and simulated results will result in better understanding of some of the vulnerabilities still present in 3D-ICs.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Nikita Podobedov

Academic Institution: Columbia University | **Major:** Biomedical Engineering

Academic Standing (Sept. '19): Junior

Future Plans (School/Career): Graduate School

NIST Laboratory, Division, and Group: PML, Microsystems and Nanotechnology Division, Biomedical Microtechnologies Group

NIST Research Advisor: Dr. Greg Cooksey

Title of Talk: Repeated Flow Cytometry Measurements Along a Single Microfluidic Channel in an Optofluidic Chip

Abstract:

High throughput measurement of cells is critical to many important areas of medicine, such as cancer screening and drug response studies. However, conventional measurement devices are limited in their capacity to combine speed and time resolution. Fluorescence microscopy can visualize single cell behavior but only with a small sample of cells and at the cost of complex analysis. Cytometers, on the other hand, have very high throughput on the order of tens of thousands of cells per second but can only take one measurement per object. This project seeks to design a high throughput cytometer that is capable of repeated and dynamic measurements. To achieve this goal, we have been testing microfluidic devices that use integrated optical waveguides to deliver excitation light and collect emission light from fluorescent materials in flow. We have focused our efforts so far on 15-micron diameter beads which contain fluorescein, a fluorophore that gives off 520 nm light. These beads are excited by a 488 nm laser while they pass through the main channel of the device, emitting light which is transmitted by internal waveguides to optical fibers and ultimately recorded by a silicon photodetector. The novelty of our devices is that they have multiple laser interrogation regions along the flow channel, each with separate detectors. This allows us to repeat measurements, validate object counting and, in general, improve measurement uncertainty. As this device is still in the very first stages of development, there are multiple issues which need to be resolved, including proper flow focusing, creating computational models to identify data uncertainties, achieving higher throughput, and, of course, switching from beads to cells. However, we are already seeing promising results with repeat measurement variation on the order of 3% between measurement regions.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Guadalupe Quirarte

Academic Institution: Harvey Mudd College | **Major:** Joint Mathematics & Physics

Academic Standing (Sept. '19): Senior

Future Plans (School/Career): Attending graduate school to pursue a PhD in applied physics

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Quantum Measurement Division, Atomic Spectroscopy

NIST Research Advisor: Dr. Joseph Tan

Title of Talk: Developing and optimizing the optical system for observing transitions between metastable states of highly charged ions created inside a mini-EBIT

Abstract:

Highly charged ions have special properties that are of interest in many disciplines including quantum information processing, development of ultraprecise atomic clocks at the one part in 10^{19} level of precision, and tests of fundamental physics. At NIST, an electron beam ion trap (EBIT) with a strong magnetic field of approximately 3 T is used to produced highly charged ions. However, there are limitations in this device that have resulted in the current development of a room-temperature, miniaturized-EBIT, or mini-EBIT. This mini-EBIT functions at a lower magnetic field of 0.29 T which is generated by using a pair of NdFeB permanent magnet rings, eliminating the use of cryogens and providing a more compact geometry. The mini-EBIT is more suitable for generating highly charged ions (HCIs) with relatively low ionization thresholds (up to around 1000 eV). Upon generating HCIs in the mini-EBIT, light emission from magnetic-dipole transitions is detected using an optical apparatus with a photomultiplier tube and counted with a multichannel scaler. We analyzed the pre-existing optical apparatus, built a truss system, and developed an optical simulation with the goal of improving robustness, minimizing light contamination, and focusing the light emitted by the highly charged ions more efficiently to the photomultiplier tube (PMT) detector within a surface area of 16.611±0.001 mm^2. By applying this procedure and implementing this revised design, new ways of intra-EBIT lifetime measurements of metastable states of highly charged ions will be explored without extracting and isolating the ions in a different ion trap. As a first test, the metastable $^2P_{1/2}$ state of Ar^{9+} $1s^22s^2\,2p^5$ will be measured and compared to the previous result of t = 9.31±0.08 ms, which was obtained by isolating the ions in a compact Penning trap.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Tojo Steven Rabemananjara

Academic Institution: University of Maryland College Park | **Major:** Computer Engineering

Academic Standing (Sept. '19): Senior

Future Plans (School/Career): Graduate School - Undecided

NIST Laboratory, Division, and Group: Physical Measurement Laboratory Division 685.11, Surface and Interface Metrology

NIST Research Advisor: Thomas Germer

Title of Talk: Camera and Projector Synchronization to Improve SI-MMI Speed and Efficiency

Abstract:

The objective of my project has been to improve the timing and light usage efficiency of our group's Structured Illumination Mueller Matrix Imaging (SI-MMI) setup comprised of a sophisticated PCO imaging camera, DLP4500 light projector, liquid crystal variable retarders, polarizers, and LVR controllers for the LCs. The system devised by our group prior to my arrival combines structured illumination, which allows for control of photon penetration depth, with Mueller Matrix Imaging, which completely characterizes a given sample's polarization properties, to achieve controlled, quantitative polarization assessment of a sample at varying tissue depths. The system used a very high camera exposure time of 100 ms in order to ensure viable image data to be used for SI-MMI analysis which resulted in an overhead of 44 seconds to acquire a full spatial frequency sweep of a sample. Neutral density filters rated from 2.5 to 6 were used to compensate for the high camera exposure time which discarded 99% of the light coming from the light projector. Our group drastically ameliorated the existing setup by abandoning the neutral density filters and instead synchronizing our camera to our projector via a trigger sent from the DLP4500 to the PCO camera. The system now uses an exposure time of no more than 50 ms, discards no light coming from the projector, and achieves a full spatial frequency sweep in around 4 seconds. The long term/ big picture goal of this project is realizing real time assessment of tissue viability in a clinical setting; application of such optical technology would be relatively inexpensive and non-invasive.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Heriniaina Teddy Rakotomanana

Academic Institution: University of the District of Columbia | **Major:** Mechanical Engineering

Academic Standing (Sept. '19): Junior

Future Plans (School/Career): Graduate school/Pursue career in research

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Division 681, Nanoscale Metrology Group

NIST Research Advisor: Andras Vladar and Kate Klein

Title of Talk: Fabrication of a Helium Ion Machined Nanochannel Device

Abstract:

The Orion Helium Ion Microscope (HIM) is capable of imaging at the sub-nanometer scale similar to a scanning electron microscope (SEM) however, the helium ions have non-negligible mass that affect the substrate. For silicon substrates in particular, we have observed that a high dose of helium, beyond normal imaging level (>10^17 ions/cm^2), results in the sputtering (removal) rate being surpassed by the implantation rate. This induces swelling deformation just below the substrate surface. These swellings eventually coalesce into nano-to-microscale internal cavities. With controlled dose and patterning, we can create custom fluidic pipe structures on the surface.

In this project, a microfluidic test chip consisting of two parallel microchannels separated by a nanochannel is fabricated in four main steps. First, the parallel microchannels and fluidic reservoirs are patterned using photolithography. Second, the microchannels are etched into the silicon substrate using KOH and resist is removed. Third, the helium-machined nanochannel is patterned between the microchannels using the HIM. Lastly, the whole device is fluidically sealed using PDMS, which is fabricated by soft lithography with a 3D printed mold. Once the device is sealed, it is tested for fluid conductivity. This work offers unique capabilities for direct-write fabrication of complex nanofluidic structures, and may lead to the acceleration of novel application discovery in energy, health diagnostics, or lab-on-a-chip microfluidics.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Holland Rhodd-Lee			
Academic Institution: Wellesley College		**Major:** Neuroscience and Music	
Academic Standing (Sept. '19):	Graduated from Wellesley College in May 2019.		
Future Plans (School/Career):	I plan on attending graduate school in the fall of 2020.		
NIST Laboratory, Division, and Group:	PML: Microsystems and Nanotechnology group		
NIST Research Advisor:	Dr. Mandy Esch		
Title of Talk:	Measuring Endothelial Molecular Transport Using a Pumpless Microfluidic System		

Abstract:

Human umbilical vein endothelial cells (HUVEC) are prominent in endothelial research. Monolayers of the cells are an ideal lab model for studying the pathology of the endothelial lining of blood and lymphatic vessels, in addition to transport of substances across cell layers. When subjected to fluidic flow they form aligned, confluent cell layers that mimic the physical and biological barriers found in vivo. This presentation focuses on the pumpless microfluidic device we have designed and developed to mimic the transport of drugs across an endothelial cell layer. We aim to demonstrate how these pumpless devices are easy to use, and allow for highly parallel operation compared to conventional pumped devices.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Amberly Ricks			
Academic Institution: Arizona State University		**Major:** Electrical Engineering	
Academic Standing (Sept. '19):	Graduate student		
Future Plans (School/Career):	Begin my masters degree in electrical engineering at Arizona State University.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Nanoscale Device Characterization Division, Nano		
NIST Research Advisor:	Dr. Emily Bittle		
Title of Talk:	Electrical Characterization of DNTT-based Organic Field Effect Transistors		

Abstract:

Organic field effect transistors (OFETs) are pursued by researchers as an opportunity to implement unique new technologies and improve cost. Organic semiconductors are competitive materials due to their structural flexibility, chemical tunability, and solution processability. These properties offer solutions to various problems posed by traditional semiconductors, specifically by the broad range of deposition methods available, including printed electronics techniques, and by the ability to better couple with other materials, including biological and curved materials. However, structure varies widely in organic semiconductors due to the diversity of molecules available; further, organic semiconductors exhibit unique transport mechanisms, making it difficult to properly implement them.

This research aims to electrically characterize OFETs based on dinaphtho[2,3-b:2′,3′-f]thieno[3,2-b] thiophene (DNTT), which is a high performing, small molecule organic semiconductor. Electrical testing compares flicker noise and "turn-on" behavior in OFETs with two different dielectric interfaces, specifically between silicon dioxide and a fluoropolymer. This characterization provides information about the trap density of charge carriers at the interface between DNTT and the dielectric. These characteristics clarify how the devices can best be implemented into useful applications and illuminate how the devices can be improved. Additionally, these parameters provide a metric for organizing and identifying these materials for future standardized use.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Russell Schwartz		
Academic Institution: The George Washington University	**Major:** Electrical Engineering	
Academic Standing (Sept. '19):	Junior	
Future Plans (School/Career):	Obtain a Master's degree in Electronics, Photonics, and MEMS	
NIST Laboratory, Division, and Group:	PML, Nanoscale Device Characterization, Alternative Computing Group	
NIST Research Advisor:	Dr. Brian Hoskins	
Title of Talk:	Closed loop update algorithm for Neuromorphic AI Accelerators	

Abstract:

Artificial Intelligence (AI) is rapidly becoming one of the most prominent fields for both research and industry. As AI tasks get more complicated computational power quickly becomes an issue, with the solution being dedicated hardware implementations for AI. Neuromorphic systems based on analog resistive memories are one such example of dedicated hardware that can be used for AI. Unfortunately, these resistive memories require sequential, one-by-one closed loop programming. Using the singular value decomposition (SVD) of the error gradient, however, we propose to implement network level closed loop training. The implementation of the closed loop SVD update was shown through simulations of a neural network using MNIST while varying hyperparameters. The hyperparameters that were varied include SVD rank, batch size, maximum epochs, and degree of nonideality with each case having the learning rate optimized to the specific set of hyperparameters. The update algorithm was then further shown on physical circuit arrays using a probe card and circuit wafers.

The results from these tests showed high rates of accuracy that were rank dependent across all degrees of nonideality. Along with this the results showed a nonlinear progression between accuracy/loss and increased SVD rank. The results of this project seems to suggest that a closed loop ranked SVD update could help to improve the Neuromorphic systems for dedicated AI usage. Along with this it also appears that there are various "best ranks" to be used in the SVD algorithm where the hyperparameter set defines the ideal rank to be used. This algorithm could also be used in conjunction with other means of increasing the computational power to further create a better overall system.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Macrae Alexander Smith		
Academic Institution: Purdue University	**Major:** Electrical Engineering	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Pursue Masters Degree	
NIST Laboratory, Division, and Group:	PML, 628, Smart Grid Testbed	
NIST Research Advisor:	Allen Goldstein	
Title of Talk:	Providing a Digital Framework for Testbed Research With LabVIEW	

Abstract:

Research is growing ever reliant on using digital systems to compliment, if not fully replace, analogue ones. However, when digital instruments are produced from different manufacturers, they are often each designed to have completely unique operating controls, making simultaneously utilizing several of these devices cumbersome. Fortunately, there exists a set of standard instrumentation application programming interfaces (APIs), the international virtual instrument (IVI) standards.

Researchers may often need to create code in order to have their testbed equipment perform specific tasks. Coding these tasks is often a time consuming process fraught with debugging, and this can all be a major hurdle that delays researchers from completing their experiments. In an effort to quickly complete their work, researchers may overlook reusability, flexibility, or robust error handling.

To help reduce the overhead needed for coding, as well as to remove the complexity of simultaneously operating several competing instrument software, an open-source LabVIEW framework is being created to be used by researchers. This IVI-compliant framework is designed to provide integrated control of all testbed equipment from one centralized hub. It is modular, highly configurable, features a robust error handling system, and can be set to automatically run experiments for the user.

In this presentation, we will be covering the concepts behind this software, the development of one of its modules, and current and future capabilities.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Hristiana Stoynova		
Academic Institution: CUNY Hunter College	**Major:** Environmental Studies	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Pursuing a career in Urban Ecology	
NIST Laboratory, Division, and Group:	PML, Sensor Science Division, Remote Sensing Group	
NIST Research Advisor:	David Allen	
Title of Talk:	Reducing Uncertainties in Carbon Storage and Fluxes: A Focus on Japanese Stiltgrass	

Abstract:

Development and agricultural expansion have created highly fragmented landscapes across the US and across the globe. In northeastern US, 23% of the forests are within only 30 meters of a forest edge. Fragmentation profoundly alters growing conditions near the edge. For example, edges experience higher temperatures and decreased soil moisture, as well increased nutrient inputs and light. These unique environmental conditions can change the vegetation growth rates and herbivory patterns, affecting both the uptake and release of CO2. However, nearly all our understanding of vegetative net primary productivity (NPP) comes from intact forests. Not accounting for fragmentation introduces uncertainties in carbon estimates and budgets.

The Forest Optical Reference for Evaluating Sensor Technology (FOREST) project uses NIST as a testbed for quantifying forest carbon dynamics in a fragmented landscape using field and remote sensing-based approaches. Solar induced florescence (SIF) instruments and methods are being developed to advance our capacities to monitor vegetative responses to environmental variations. We empirically characterize the physiological and ecological meaning of SIF by directly linking to carbon exchange from ground measurements across the different land cover types of the NIST campus. NIST houses a large deer population, as commonly found in fragmented and suburban landscapes. The deer inhibit forest regeneration by eating tree seedlings and sapling, creating optimal conditions for invasive species such as Japanese stiltgrass (Microstegium vimineum). In the absence of saplings, the stiltgrass becomes the only source of understory NPP, but its rates of productivity are unknown. This project utilizes the NIST FOREST site to quantify rates of carbon sequestration by Japanese stiltgrass and its contribution to carbon dynamics in fragmented suburban forests. We integrate field measurements of productivity with forest understory light dynamics and near-surface remote sensing of vegetation indices to quantify understory contributions.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Ben Wade		
Academic Institution: University of Maryland, College Park	**Major:** Physics and Astronomy	
Academic Standing (Sept. '19):	Senior	
Future Plans (School/Career):	Attend graduate school in physics or astronomy	
NIST Laboratory, Division, and Group:	Physical Measurements Laboratory, Nanoscale Device Characterization Division, Nan	
NIST Research Advisor:	(Charles) Kin Cheung, Pragya Shrestha	
Title of Talk:	High Bit Rate Solid State Quantum Random Number Generation	

Abstract:

Random number generation is an integral part of many cryptographically secure applications. Because these applications are so widespread in the digital age, sources of random numbers play a very important role in technology. Commonly used pseudo-random number generators rely on preset algorithms and are consequently not truly random. This serves as a security risk. However, quantum-based phenomenon are believed to be truly random. We aim to leverage noise produced by quantum transitions in resistive random-access memory (ReRAM) to produce true random numbers. Due to the massive amount of information to encrypt, a generator capable of producing many outputs in a short amount of time is ideal. Similar work in the past have demonstrated generators that do not have a sufficiently high bit rate. ReRAM devices show high-speed operation at low power and are of a simple design, making them ideal candidates to work with. My task is to determine the randomness of the fluctuations they generate. I do so for a series of ReRAM devices and test their combined output using a statistical suite designed by NIST. Consisting of 15 tests, the suite examines several properties of the sequence, such as the entropy of the overall system. I encode the test suite using Python and run the battery of tests on data obtained from the devices. From these tests I can determine whether ReRAM is a viable source of true random numbers for use in secure encryption.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Hunter Wages		
Academic Institution: Wofford College	**Major:** Mathematics and Physics	
Academic Standing (Sept. '19):	Graduate School at Wake Forest	
Future Plans (School/Career):	PhD in Applied Mathematics	
NIST Laboratory, Division, and Group:	PML, Sensor Science Division, LBIR group	
NIST Research Advisor:	Solomon Woods	
Title of Talk:	Thermal Imaging: An End-to-End Simulation	

Abstract:

Currently, there is no non-invasive method for creating a 3-dimensional image of the temperature distribution throughout a volume. Using multi-layer magnetic nanoparticles (MNP) 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. However, to accomplish this with accuracy, a very sensitive and specific magnetic field sensing system must be designed and implemented. This summer, we have created an end-to-end model and simulation of the experiment, in order to optimize the setup of the magnetic field sensing system and obtain theoretical expectations for the accuracy of these measurements.

In setting up this simulation, there were three key areas in which the model had to be understood: 1) the relationship between the temperature of the MNP and its magnetization, 2) the relationship between the orientation of the sample magnetization and the magnetic flux through the sensor, and 3) the relationship between the geometry of the electromagnet coils and/or permanent magnets and the spatial dependence of the magnetic field generated at the sample. In order to complete the simulation, we used a combination of modeling in COMSOL, MATLAB, and solving electromagnetic problems analytically. This work has helped in the optimization of the experimental setup for obtaining the most sensitive temperature measurement and best spatial resolution.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 5-9, 2019

Name: Eli Weissler		
Academic Institution: Harvey Mudd College	**Major:** Physics	
Academic Standing (Sept. '19):	Graduated May '19	
Future Plans (School/Career):	I plan to work as a scientist at Areté Associates	
NIST Laboratory, Division, and Group:	Physical Measurement Lab, Quantum Measurement, Quantum Optics Group	
NIST Research Advisor:	Zachary Levine	
Title of Talk:	Photon Echo Based Quantum Memory	

Abstract:

Quantum networks have the potential to revolutionize secure communication by encoding information in the properties of individual light particles, i.e., photons. One of the biggest challenges in building these networks is sending quantum-correlated, or entangled, photons over long distances. To be effective, there needs a high degree of entanglement, but these correlations decay exponentially with distance over existing fiber-optic channels. Researchers have proposed using special repeaters to boost entanglement along the way, but they require a "quantum memory" that can store individual photons with little to no loss. No such device exists today.

We model a memory based on "photon echos" which has the potential to create a device good enough for use in a repeater. In a photon echo, light incident upon a specially prepared crystal is echoed back after some amount of time that we can control. Using a mixture of quantum mechanics and classical electrodynamics, we hope to understand the phenomenon and help guide our experimental collaborators at the University of Maryland, who are currently implementing a photon echo memory using Praseodymium-doped Yttrium-Orthosilicate.

Our results indicate that the most important step in the preparation is using a frequency modulated laser to manipulate the electronic states of the Praseodymium into an "atomic frequency comb." Our work highlights the importance of periodicity of phase, as well as amplitude, of the driving pulse and promises to optimize the spectral content of the modulation to make better combs and create them faster.

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First Name	Last Name
Samantha	Gibson
Sue	Lee

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NIST- Gaithersburg, MD
August 5-9, 2019

Name: Samantha Gibson	
Academic Institution: The University of Arkansas at Pine Bluff	**Major:** Biology
Academic Standing (Sept. '19):	Senior
Future Plans (School/Career):	Purse and M.D./Ph.D. in Biomedical Engineering.
NIST Laboratory, Division, and Group:	Technology Partnerships Office (TPO) and Technology Discovery Office (TDO)
NIST Research Advisor:	Paul Zielinski
Title of Talk:	Technology transfer development at NIST and the Technology Discovery Office

Abstract:

The mission of NIST's Technology Partnerships Office (TPO) is to promote US competitiveness, for National Institute of Standards and Technology (NIST) and the Department of Commerce (DOC). TPO arranges agreements called Cooperative Research and Development Agreements (CRADAs) to aid collaboration with non-federal parties, manages NIST intellectual property such as patents and licenses, key player in enabling the commercialization of NIST R&D. In August 2018, NIST established the Technology Discovery Office (TDO) to focus on improving the discoverability of NIST research. TDO's goals are to create a NIST scientist profile system, produce executive summaries on NIST inventions, and compile weekly tech transfer news articles. Several biography websites and profile tools were compared to determine necessary requirements and complementary features of the NIST profile system. A comparative analysis of existing solutions was performed to narrow down the products and forms were filled out for NIST scientists to place information inside of a database allowing them to be found easier. Creation of executive summaries enables NIST's ability to inform companies and manufacturers about the benefit of the new inventions. Weekly reports on technology transfer news and event reports are created to provide information on the newest technology transfer information to NIST scientists and the public. With the mission of enhancing the discovery of NIST research and technologies by government, industry, academia, and the general public, and assisting technology transfer leading to commercialization, we have contributed to the development of the TDO in its early stages. In completion, there was a connection established between NIST scientists and the public, economic opportunities could be created, and possible life-saving technology transfer opportunities became easily accessible.

SURF Student Colloquium

NIST- Gaithersburg, MD
August 5-9, 2019

Name: Sue Lee	
Academic Institution: Carnegie Mellon University	**Major:** Computer Science
Academic Standing (Sept. '19):	Sophomore
Future Plans (School/Career):	Pursuing a Career in Human Computer Interaction
NIST Laboratory, Division, and Group:	Technology Partnerships Office, Technology Discoverability Office
NIST Research Advisor:	Paul Zielinski
Title of Talk:	Technology Transfer Development at NIST and the Technology Discovery Offi

Abstract:

The mission of NIST's Technology Partnerships Office (TPO) is to promote US competitiveness, for National Institute of Standards and Technology (NIST) and the Department of Commerce (DOC). TPO arranges agreements called Cooperative Research and Development Agreements (CRADAs) to aid collaboration with non-federal parties, manages NIST intellectual property such as patents and licenses, key player in enabling the commercialization of NIST R&D. In August 2018, NIST established the Technology Discovery Office (TDO) to focus on improving the discoverability of NIST research.

TDO's goals are to create a NIST scientist profile system, produce executive summaries on NIST inventions, and compile weekly tech transfer news articles. Several biography websites and profile tools were compared to determine necessary requirements and complementary features of the NIST profile system. A comparative analysis of existing solutions was performed to narrow down the products, and forms were filled out for NIST scientists to place information inside of a database allowing them to be found easier. Creation of executive summaries enables NIST's ability to inform companies and manufacturers about the benefit of the new inventions. Weekly reports on technology transfer news and event reports are created to provide information on the newest technology transfer information to NIST scientists and the public.

With the mission of enhancing the discovery of NIST research and technologies by government, industry, academia, and the general public, and assisting technology transfer leading to commercialization, we have contributed to the development of the TDO in its early stages. In completion, there was a connection established between NIST scientists and the public, economic opportunities could be created, and possible life-saving technology transfer opportunities became easily accessible.


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