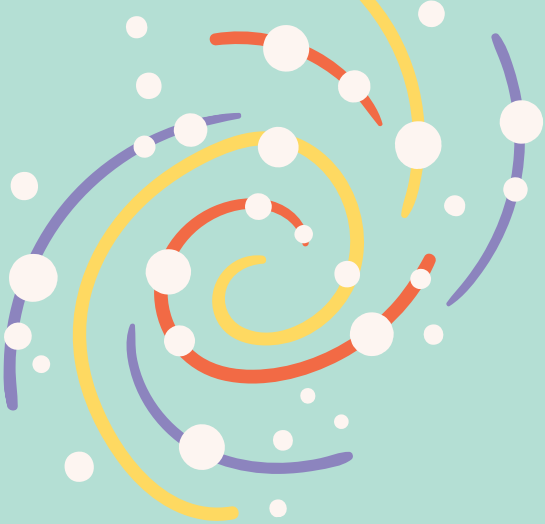
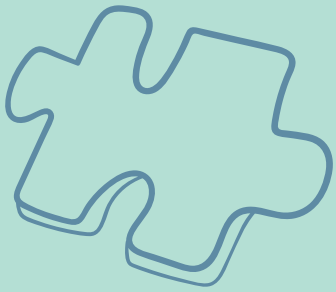
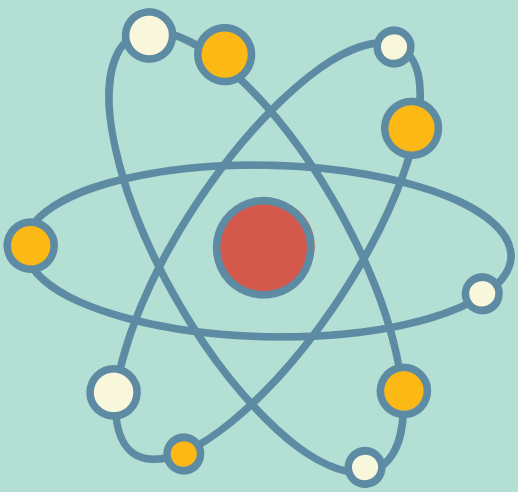




NIST | SUMMER UNDERGRADUATE RESEARCH FELLOWSHP

SURF 2023



Greetings,

On behalf of the Director's Office, I proudly present the 2023 SURF Colloquium book. Using a hybrid format, the 2023 SURF Colloquium featured in-person and virtual presentations and attendees.

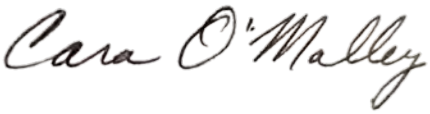
Founded by scientists in the Physics Laboratory (PL) with a passion for STEM outreach, the SURF Program has grown immensely since its establishment in 1993. SURF's first cohort consisted of twenty participants from 8 universities who conducted hands-on research primarily in the physics lab. The 2023 cohort, representing all STEM disciplines, included 172 participants from 74 universities working on research projects on the NIST campuses in Boulder, CO, and Gaithersburg, MD, and remotely. Participants from both campuses engaged in activities collectively, including the Colloquium. In the future, the program will likely include virtual and in-person components. The nation’s workforce is changing, and we must adapt.

As you peruse the Colloquium book, you are bound to find topics that pique your interest. You are welcome to email the NIST research advisors about your questions and comments regarding the ongoing research in a specific NIST laboratory. Most staff and scientists are excited to exchange findings and new ideas and love to talk about their roles and research at NIST.

I could not conclude this letter without mentioning the individuals who make the SURF Program possible. Thank you to the Lab SURF Directors, the SURF mentors, the administrative staff, OISM, and all the staff who play an integral role in creating valuable experiences for the SURF participants. Also, a huge thank you goes out to the participants, their families and friends, and the ambassadors who spread the word about SURF. Your hard work and support are greatly appreciated.

I hope you enjoy the 2023 Colloquium book and learn something new about the nation’s standards laboratory.

Best regards,



Cara O'Malley

NIST SURF Program Director

## NIST SURF Program Team

| Organizational Unit (OU) | Name |
|---|---|
| Director's Office | Cara O'Malley* |
| Director's Office | Kara Robinson |
| Director's Office | Linda Derr* |
| Communications Technology Lab | Wesley Garey |
| Communications Technology Lab | David Griffith |
| Communications Technology Lab | Lotfi Benmohamed |
| Diversity, Equity, and Inclusivity Office | Juan Fung |
| Engineering Lab | Cartier Murrill |
| Engineering Lab | Shonali Nazare |
| Information Technology Lab | Timothy Burns |
| Information Technology Lab | Yolanda Bursie |
| Information Technology Lab | Michaela Iorga |
| Information Technology Lab | Derek Juba |
| Information Technology Lab | Ian Soboroff |
| Material Measurement Lab | Katherine Gettings |
| Material Measurement Lab | Nathan Mahynski |
| Material Measurement Lab | Jessica Staymates |
| NIST Center for Neutron Research | Julie A. Borchers |
| NIST Center for Neutron Research | Leland Harriger |
| NIST Center for Neutron Research | Susana Teixeira |
| Physical Measurement Lab | Uwe Arp |
| Physical Measurement Lab | Michael Berilla |
| Physical Measurement Lab | Maritoni Litorja |
| Physical Measurement Lab | Matthew Pufall* |
| Physical Measurement Lab | Richard Steiner |
| Physical Measurement Lab | Thomas “Mitch” Wallis* |
| Advanced Manufacturing | Lisa Fronczek |
| | *based in Boulder, CO |

# Table of Contents

## August 1, 2023 - Plenary Session

| August 1, 2023 | | SURF Colloquium N1ST Plenary Session |
|---|---|---|
| | | Gaithersburg Green Auditorium & Boulder Auditorium & Virtual |
| https://bluejeans.com/334112944/3419?src=join_info | | |
| **Time (ET)** | **Agenda** | |
| **9:20 AM** | **Welcome and Moderator**<br>**Cara O'Malley**<br>**Bluejeans Moderator: Katherine Gettings** | **Title of Talk** |
| **9:30 AM** | ***EL - Anabel Kadri (Gaithersburg)*** | Degradation Mechanism and Failure Mode of Polymeric Backsheets used in Photovoltaics |
| **9:55 AM** | ***NCNR - Ethan Gasper (Gaithersburg)*** | Effects of solvents on the assembly of nanoparticles from poly(styrene-b-ethylene glycol) |
| **10:20 AM** | ***MML - George Sellers (Gaithersburg)*** | Using Electron Microscopy To Determine The Structure Of A Flexible Protein |
| **10:45 AM** | ***CTL - Nathan Gonzalez (Boulder)*** | Homodyne Tomography for Characterization of Non-classical Optical States in Quantum Networking |
| **11:10 AM** | **BREAK** | |
| **11:25 AM** | ***BOULDER - Jessica Gerac (Boulder)*** | Reproducibility in 3D Photopolymer Printing |
| **11:50 AM** | ***DEIO - Ayomide Johnson (Gaithersburg)*** | Beyond words: Examining implicit social expectations in job descriptions for Computer and Information Science positions |
| **12:15 PM** | ***ITL - Katherine Harvey (Gaithersburg)*** | Reaction Limited Approximations of Biosensor Field Effect Transist |
| **12:40 PM** | ***PML- Seoyoung Joo (Gaithersburg)*** | A real and k-space imaging spectroscopy setup for nanophotonic device characterization |

## August 1, 2023 - Parallel Sessions

| **Gburg Lecture Room C;**<br>**Boulder Bldg 1, Rm 1107** | **Gburg, Bldg 101, LR D;**<br>**Boulder Bldg 2, Rm 0113** | **Gburg Heritage Room;**<br>**Boulder Bldg 1, Rm 1203D (8-10 people)** |
|---|---|---|
| https://bluejeans.com/334112944/3419?src=join_info | https://bluejeans.com/333872104/1874?src=join_info | https://bluejeans.com/956426680/5621 |
| **EL**<br>**Moderator: Samuel Veras**<br>**Bluejeans Moderator:** | **MML**<br>**Moderator: Becky Steffen**<br>**Bluejeans Moderator:** | **PML**<br>**Moderator: Emily Bittle**<br>**Bluejeans Moderator:** |
| | | |
| *Rohan Hadavale* : Risk and Uncertainty in Community Resilience Planning | *Grace Finch:* Replacing Sanger Sequencing with Next Generation Sequencing for Variant Allele Characterization | *Jacques Deroin* : COMSOL Simulations of Electromagnetic Test Structures |
| *Kristin Dan* ***(virtual):*** Determining a Built Infrastructure Vulnerability Index | *Abigail Antonishek:* Quantitative and Qualitative Analysis of Lipid-Encapsulated mRNA | *Daniel Harrington:* Polymer Passivation of 2D TMD Photodetectors |
| *Hayley Pinkowitz:* Improving Technical Communications for the Engineering Laboratory | *Lily Min:* Digital PCR Assay Development for AAV Reference Materials | *Jarlem Lopez Morel:* Organic Electrochemical Transistors with a Gold Nanoparticle-Doped Polymer Channel |
| *Dhruv Rajagopal:* Using Comsol to Simulate Viscoelastic Fluid Motion Between Two Plates | *Sophie Lipshutz:* How to protect cells during bioprinting | *Audrey Pechilis:* Transient Absorption Spectroscopy of Exciton-Polaritons in Organic Crystals |
| | | |
| **EL**<br>**Moderator: Joannie Chin**<br>**Bluejeans Moderator:** | **MML**<br>**Moderator: Zhiyong He**<br>**Bluejeans Moderator:** | **PML**<br>**Moderator: Christine McGinn**<br>**Bluejeans Moderator:** |
| | | |
| *Janelle Davis:* Study of Pyrrhotite Reactions In Concrete | *Lukas Marple:* Advancing Metabolomics: How can we Improve Fecal Metabolite Extraction? | *Nathaniel Lawson:* Advanced charge pumping techniques for defect detection and characterization in MOSFETs |
| *Caden Williams* : Microscopy and Water-to-Cement Ratio of Concrete | *Megan Nguyen:* Investigation of the Relationship Between Diet and the Human Gut Microbiome | *Benjamin Tran:* DC Power and Energy Calibrations to Verify Electric Vehicle Supply Equipment Meters |
| *Samuel Chen* : Early Strength Development of Quick Setting Cement Mixtures | *Maria Lindsey:* Comparison of Traditional In Vitro Viability Assays | *Bryan Rezende:* Development of the calibration service for level 3 direct current (DC) power energy meters |
| *Katherine Biernacki:* Exploring the Effect of Polyethylene Terephthalate Replacements in Portland Cement Mixtures | *Jennifer Li:* Development of visualizations for the Genome In A Bottle data portal | *Andrew Peters:* The Missing Link: Automation of Magneto-Optical Spectroscopy of Quantum Materials |
| *Matthew Kubas:* Validation of the Reciprocity Law in the NIST 6-Port SPHERE Using Polyethylene Terephthalate | *Jane Jou:* Detection of EML4-ALK Fusion Cancer Biomarker in Liquid Biopsy by EFIRM | *Brady Egleston:* Characterizing 39K MOT clouds with Neural Networks |
| | | |
| **EL**<br>**Moderator: Cartier Murrill**<br>**Bluejeans Moderator:** | **MML**<br>**Moderator: Alex Landauer**<br>**Bluejeans Moderator:** | **PML**<br>**Moderator: Charles Clark**<br>**Bluejeans Moderator:** |
| | | |
| *Leon Zhang:* A Review of Public Radio Usage for Risk, Crisis, and Disaster Communication | *Walter Adamy:* Comparison of High-Rate and Quasi-Static Mechanical Testing for Aged and Unaged Single High Strength Fibers for Use in Body Armor Applications | *Noah Zuckman:* Analysis of test data from the portable EBIT for NIST Boulder |
| *Eric Fagan* ***(virtual)*** *:* Development and Utilization of a Database on Nonstructural Component Damage | *Ryan Punith:* Mechanical Testing of Heterogenous, Graded Impact Protection Materials | *Joshua Young:* Development of an Ultrasonic Calorimeter for Dose Rate Imaging |
| *Varadraj Chavan:* Breaking Down Plastics: Unveiling the Degradation Process | *Bradlee Rich:* Solving the worlds textile waste problem one blend at a time | *Alisha Patel:* Analyzing the Effects of V-Vial Parameter Changes on Ionization Chamber Response Using TOPAS |
| *Braedon Mullin:* In-Situ Calibration of Differential Pressure Transducers | *Max Mevorah:* Synthesis and Characterization of Metal-Impregnated Lewatit for Direct Air Capture (DAC) | *Ethan Zheng:* The modelling and testing of the Wide Angle Free Air Chamber |

# August 2, 2023 - Parallel Sessions

| Gburg Lecture Room C;<br>Boulder Bldg 1, Rm 1107 | Gburg, Bldg 101, LR D;<br>Boulder Bldg 2, Rm 0113 | Gburg Heritage Room;<br>Boulder Bldg 1, Rm 1203D (8-10 people) |
|---|---|---|
| https://bluejeans.com/334112944/3419?src=join_info | https://bluejeans.com/333872104/1874?src=join_info | https://bluejeans.com/956426680/5621 |
| **EL**<br>**Moderator: Jason Averill**<br>**Bluejeans Moderator:** | **MML**<br>**Moderator: Christopher Sims**<br>**Bluejeans Moderator:** | **ITL**<br>**Moderator: Tim Burns**<br>**Bluejeans Moderator:** |
| | | |
| *Bradley Estacio* ***(virtual)*** : Efficient and Compliance Check of HVAC information for Two NIST Facilities | *Tyler Hicks:* Exploration of Parameters for Carbon Nanotube Separations via Automated Fluorescence Titration | *Vivian Xiao:* BioFET Sensitivity Analysis |
| *Robert Carlyon:* Predicting Wildfire Spread using Computational Fluid Dynamics | *Colin McCarragher:* Analysis of Polyzwitterion Solutions Using Dynamic Light Scattering | *Luke Hawranick:* Inter-node Communication Performance Tuning |
| *Jaskaran Gill* : Online Documentation for NIST Fire Dynamics Simulator (FDS) | *Gabrielle Schumacher:* Liquid Crystal Elastomer Membranes for Enhanced Impact Resistance of 3D Structures | *Dongxing He:* Fiber-link characterization of quantum network fibers using single photon detection. |
| *Tiller Van Doren:* Fire Research Problem: Construction of Flame Spread Apparatus | *Mia Merritt:* Study of Iron Oxide Nanoparticle Dynamics Based on Surface Functionalization for Magnetic Particle Imaging | *Michael Szilagyi:* Converting OpenGL Shaders to Run in ParaView Visualization Software |
| *Nicholas Redford:* Interpolation of Flammability Behaviors through Different Materials | *Muhammad Rafi:* Developing a spectral accurate solution to assess results for the Cahn-Hilliard benchmark | *Morgan Ko:* Making 3D Formats Accessible for Scientific Data Using glTF |
| | | |
| **EL**<br>**Moderator: Christine Beyzaei**<br>**Bluejeans Moderator:** | **MML**<br>**Moderator: Daniel Wines**<br>**Bluejeans Moderator:** | **ITL**<br>**Moderator: Tim Burns**<br>**Bluejeans Moderator:** |
| | | |
| *Yehoshua Halle* : Digital Twin Development for an Automated Robot Workcell | *Spencer Mattes:* Temperature and pressure dependence of dielectric spectra based on molecular dynamics simulations | *Leon Jia:* Characterization of Quantum memories and SiC-based Quantum Devices |
| *Ivon Charlery* : Digital Twin of Desktop Computerized Numerical Control Machine | *Nishwanth Gudibandla:* Understanding the Magnetic Properties of 2D Vanadium Diselenide with Density Functional Theory | *Mikhail Krepets:* Modifying the Walk on Spheres algorithm to see if it would make ZENO faster. |
| *William Stiller* : Hierarchical Data Structure Development to Support Digital Thread and Digital Twin Applications | *Aubrey Augustine:* Assessing Magnetic Levitation for Plastics Densimetry | *Faadil Shaikh:* Implementation of Fastest Closest Point in the West to accelerate Capacitance calculations using ZENO |
| *Vladimir Alvarado* : Using Large Language Models to Help Formulate Scheduling Problems | *(virtual) Leila Rose Clark:* Investigating Shear-Induced Disentanglement Using the Slip-Link | *Thomas Wolcott:* Designing an interface for the B-Spline R-matrix codes |
| *Tali Schlenoff* : InterFace the Facts | *Leonardo Borchert:* Optimization of Nano-Calorimetry Sensors using Finite Element Simulations | *Peter Burbery* ***(virtual)*** : Translating Mathematica expressions in q-calculus to LaTeX |
| | | |
| **EL**<br>**Moderator: Aron Newman**<br>**Bluejeans Moderator:** | **MML**<br>**Moderator: Russell Maier**<br>**Bluejeans Moderator:** | **ITL**<br>**Moderator: Michaela Iorga**<br>**Bluejeans Moderator:** |
| | | |
| *Parker Liposky:* Aerial Drop Test Research | *Connor Davison:* Improving Toughness of Ceria-Based Oxygen Ion Conductors | *Noah Schulman:* Evaluating Generative AI Audio Deepfake Tools |
| *Ethan Sundel:* Standardized Testing and Validation of Emergency Response Systems | *Alison Hecht:* Exploration of diblock copolymer blend thin films to understand multicomponent system morphologies | *Kaylin Yeoh: An Evaluation of Synthetic Data Generation Methods for Tabular Data* |
| *Brian Maloney:* ROS Integration with Agile Performance Robotic Systems | *Evan Freeland:* Thickness Measurement of Gallium Phosphide Films on Silicon with Micro-X-Ray Fluorescence | *Luke Zic:* Video Retrieval Evaluation Leaderboard Development |
| *Khoa Nguyen:* Collection, Analyzation, and Vizualizing of RGB and Depth Data for Human Study | *Arden Dombalagian:* Nanocalorimetry for Carbon Capture Materials Characterization | *Marilyn Nguyen:* Implementations of Mobile Driver's Licenses and Everyday Documents |
| *Noam Peled:* Real-time Pose Measurement to Support Robot Inspection | | *Alex Dai:* Exploring Suitable Structures to Store mDoc Field Data. |

# August 2, 2023 - Parallel Sessions (continued)

| **CTL (+1 EL)**<br>**Moderator: CTL: David Griffith**<br>**Bluejeans Moderator: EL: Cartier P Murrill** | **MML**<br>**Moderator: Brian DeCost**<br>**Bluejeans Moderator:** | **ITL**<br>**Moderator: Michaela and Nikita**<br>**Bluejeans Moderator:** |
|---|---|---|
| | | |
| ***EL*** *- Elijah Martin:* Developing a Custom Spin Coater Using a Microcontroller and 3D printing | *Ryan Kim:* AELF multiagent machine learning to map transfer data | *Brian Chen* ***(virtual)*** *:* Graph Database for NIST Cybersecurity Publication Citation Relationships |
| ***CTL*** *- Benjamin Philipose:* Integrating Network Simulations for Enhanced Vehicle Performance Analysis | *Dennis Zhao:* Analyzing phase diagrams using machine learning | *Jayden Crosby* ***(virtual)*** *:* Chatbots and Search |
| ***CTL*** *- Benjamin Winig:* Simulating Manufacturing Environments with SimPROCESD | *Tristan Charles:* Utilizing Machine Learning to Analyze Carbon Dioxide Capture Efficiency | *Francsi Durso* ***(virtual)*** *:* A Combinatorial Approach to Explainable AI |
| [redacted] | *John Marquart:* Similarity Metrics applied to Neural Networks: Examining how Material Properties are Learned | *Navya Gautam* ***(virtual)*** *:* Creating an Enriched Cybersecurity Risk Dataset with Visualizations to Analyze and Evaluate Cyber Risk Incidents |
| | *Andrew Celi:* Integrated NIST Knowledge Website | *Anthony Malysz* ***(virtual)*** *:* "Next Generation Policy-as-Code" |

| **PML**<br>**Moderator: Susana Deustua**<br>**Bluejeans Moderator:** | **MML**<br>**Moderator: Meagan Cauble**<br>**Bluejeans Moderator:** | **ITL**<br>**Moderator: Nikita Wooten**<br>**Bluejeans Moderator:** |
|---|---|---|
| | | |
| *Travis White:* Analyses in Laboratory Metrology | *Jay Kannan:* Using the WIPP System for Imaging Cell-Virus Interactions | *John Guerreio* ***(virtual)*** *:* Understanding Memory-Related CWE Entries with Bugs Framework |
| *Dinelka Jagoda:* Educational Outreach Resources | *Sheetal Padhi:* Containerized Tools for Image Processing and Analysis of Live Induced Pluripotent Stem Cells | *Zach Benton* ***(virtual)*** *:* CNN-based texture directionality detection |
| *Jeremy Robin:* Multiplexed Electrochemical Biosensing | *Carina Delcore:* An Investigation of Arginine-rich Antimicrobial Peptides and their Interactions with Lipid Membranes | *Vidhata Jayaraman* ***(virtual)*** *:* Surprising Sentences |
| *Ginny McCracken:* Fabrication and Characterization of Functionalized Graphene Field Effect Transistor for the Quantification of Exosomes Produced by Induced Pluripotent Stem Cell-Derived Cardiomyocytes | *Jonah Oxman:* Characterizing Antibody Flexibility: 2D Codistribution Analysis of Disulfide Bond Reduction | [redacted] |
| *Connor Skelton:* Uncertainty Quantification in Flow Cytometry with AM Modulation | *Sragvi Pattanaik:* Exploring the Role of Bacterial Motility in Evolutionary Mechanisms for Antimicrobial Resistance | |

# August 3, 2023 - Parallel Sessions

| Gburg Lecture Room B;<br>Boulder Bldg 1, Rm 1107 | Gburg, Bldg 101, LR D;<br>Boulder Bldg 2, Rm 0113 | Gburg Heritage Room;<br>Boulder Bldg 1, Rm 1203D (8-10 people) | Gburg, Bldg 101, LR C ;<br>Boulder - Bldg 81, Rm 1A-116 |
|---|---|---|---|
| https://bluejeans.com/334112944/3419?src=join_info | https://bluejeans.com/333872104/1874?src=join_info | https://bluejeans.com/956426680/5621 | https://bluejeans.com/348888487/9420 |
| **PML**<br>**Moderator: Maria Nadal, Daniel Barker**<br>**Bluejeans Moderator:** | **MML**<br>**Moderator: Howie Joress**<br>**Bluejeans Moderator:** | **ITL**<br>**Moderator: Derek Juba**<br>**Bluejeans Moderator:** | |
| | | | |
| *Olivia Green:* Testing the performance of optomechanical pressure sensors | *Kira Corning:* Generation of a Rapid GC-MS Library for Fire Debris Analysis and Ignitable Liquid Identifications | *Ishaan Bhardvaj:* Impact of Weather Parameters on Path and Clock Delay in Quantum Networks | |
| *Benjamin Baldwin:* Rotational Cooling of a Molecular Beam | *Nikhila Narayana:* Compilation and Evaulation of Temperature Reference Points for the Alkali Metals | *Kathryn Butziger:* Comparison of AI Model Attribution Methods | |
| *Gabriel Kuntz:* Developing a robust and cost-effective digital PID controller for laser cooling | *Raine Antonio:* Bubble Trouble - Identification of Defect Sites in Glasses Using Optical Microscopy | *Carina Carino:* Deep Learning-Based Viral Plaque Detection in Label-Free Phase Contrast Images | |
| *Grace Waters:* Measuring the Bidirectional Reflectance of Materials for UVC Germicidal Applications | *Jacob Blinkoff:* Modeling Chloride Diffusion in Concrete | *Ryan Trask:* Correction of the Meniscus Effect in Biological Samples with Convolution Neural Network Models | |
| *Rishabh Sinha:* Simulation and Measurement of 3D Thermal Gradients in Liquids for Magnetic Imaging Validation | *Sarah Lehrman:* Determining the yield stress and frequency dependence of printable thermoset composite resins | *Stanley "Troy" Conklin:* Creating Abstractions for Real-time Image Processing | |

| **PML**<br>**Moderator: Joe Rice**<br>**Bluejeans Moderator:** | **NCNR**<br>**Moderator: Dr. Guebre Tessema, National Science Foundation**<br>**Bluejeans Moderator:** | **ITL**<br>**Moderator: Derek Juba**<br>**Bluejeans Moderator:** | **Boulder SURF Participants**<br>**Moderator: Ellen Meyer**<br>**Bluejeans Moderator: Adam Keim** |
|---|---|---|---|
| | | | |
| *Dawn Pierce:* Measuring the UV Transmittance of DMDs and How It Will Help Us Search for Habitable Exoplanets | *Patrick Chen:* Simulating Domain Walls in Weyl Semimetals to Study the Effects of Weyl Fermions on Magnetic Behavior | *Sonika Sharma:* Confirm That 25 747 New Programs Can Replace the 32 003 Programs of the Old C# Test Suite | |
| *Briana Chen:* Measuring digital micromirror device characteristics in the infrared wavelength regime | *Kimia Samieinejad:* Chemical Vapor Deposition of Uranium Ditelluride (UTe2) | *Saahil Singh:* Mapping Categorical Emotions and Dimensional Attributes from Text Data to | |
| *Colleen Ewald:* Impact of the Degradation rate of Photodiodes on CANDLE Project | *Justin Wang:* Reinforcement Learning and Spin Waves | *Max Filliben:* Web-based Statistical Tools for Radionuclidic SRMs | |
| *Amanda Younes:* Rydberg atom sensing of blackbody radiation | *Navid Misaghian :* Harmonizing Human-Machine Interfaces: A Standard Reference Guide for HMI Design and Management at the NCNR | *David Sadek:* Errors in Variables Regression Models | |
| | *Amir Dajani:* Development of a Validated CFD Model for the Mixing Behavior of Parallel Triple-Channel Flows | *Femina Amoo:* Evolution of cybersecurity education and workforce development | *Jake Shin:* High Resolution Light Scattering Measurements of Information Displays |
| | | | *Grant Mondeel* : A Real-Time Data Analysis GUI for Transition-Edge Sensor Array Spectrometers |
| | | | *Jacob Stuligross:* Software to Support Gamma-ray Spectrometry |
| | | | *Ethan Sontarp* : Molecular Dynamics Simulations of Aqueous NaF using Polarizable Force Fields |

| **PML**<br>**Moderator: Zachary Levine**<br>**Bluejeans Moderator:** | **NCNR**<br>**Moderator:**<br>**Bluejeans Moderator:** | **ITL**<br>**Moderator:**<br>**Bluejeans Moderator:** | |
|---|---|---|---|
| | | | |
| *Addhyaya Sharma:* Assembling DNA origami fused plasmonic nanopores for single molecule detection | *Kaitlyn Esneault:* Sample Development for Small Angle Scattering and Neutron Interferometry | | *Essa St George:* Laser Scanning Microscope for High-Speed Waveform Metrology |
| *Ziran Du:* Saturation of Susceptibility in a Two-Level System, a Model of a Rb Vapor Cell | *Sanjana Sureshbabu* : Constructing Native Extracellular Scaffolds for Tissue Repair | | *Anh Katherine Le:* Clock Data Analysis Using Least Squares and Allan Variance Techniques |
| *John Taylor:* Examining the Experimental Limitations of the Quantum Ampere | *Surabhi Singh:* Understanding Mitochondrial Dysfunction Through Structures of Cardiolipin-Bound Cytochrome c in Healthy and Pathological Model Membranes | | |
| *Mya Merritt:* Obtaining Super Resolution with Thermal States using Photon Number Resolving Camera | *Rahil Verma:* Optimizing Pharmaceutical Formulations | | |
| *Justin Craven:* Faster ultracold atom data collection through the use of a one-dimensional optical molasses | **END of NCNR *SURF* presentations** | | |

## August 3, 2023 - Parallel Sessions (continued)

| NCNR *CORE*<br>**Moderator:**<br>**Bluejeans Moderator:** | **Boulder SURF Participants**<br>**Moderator: Jacob Stuligross**<br>**Bluejeans Moderator: Grant Mondeel** |
|---|---|
| *Thomas Murray:* Molecular Mass and Composition Dependence of Glass Transition Temperature in PC/PMMA Blends | *Adam Keim :* Cryogenic low-noise DC measurements of nanoscale Josephson junctions |
| *Eugene Jeong:* Strain-mediated parallel to antiparallel magnetization reorientation in Co/Cu multilayers | *Tuan Anh Nguyen:* Characterizing extended InGaAs photodiode shot noise at 4 K |
| *Christopher Lipscomb:* Building a Master Equipment List for the National Bureau of Standards Reactor | *Matthew Rilloraza:* Frequency Comb Calibrated Laser Heterodyne Radiometry for Precision GHG Measurement |
| *Nelay Sharma:* Building & Establishing a database enterprise management system | *Anthony Adesso* : Accessible smartphone-based pH sensors using magnetic hydrogels |
| *Duncan Beauch:* Development of an Interface to Accelerate MCNP Reactor Simulations | *Victor Lita:* Optimizing Electrochemical Reactions for Microwave Microfluidic Analysis |
| *Evan Bures* (virtual): Exploring the Potency of Computational Fluid Dynamics for Holistic Reconstruction of flow behavior in the NIST Neutron Design | *Kayla McCreary:* Comparing THC Recovery from Impaction and Electrostatic Filter Devices |
| | **Boulder SURF Participants**<br>**Moderator: Victor Lita**<br>**Bluejeans Moderator: Ethan Sontarp** |
| | *Natalie Bruhwiler:* Radio frequency induced heating of passive implants during low field MRI |
| | *Kamakshi Subramanian:* MRI of Tumor Mimics with Quantitative and Radiomic Analysis |
| | *Ellen Meyer:* Robotic Calibration for Scales Used to Measure Radiation Pressure |
| | *Ernesto Flores:* Measuring Metal-Melting Lasers at their Focus |
| | *Eve Blank:* Pareto Tracing Ridge Profiles for Wind Turbine Design |
| ***THANK YOU!*** | |


# Boulder, CO
# 2023

## Summer Undergraduate Research Fellowship (SURF) - 2023 Participants

*(in the order of the Colloquium schedule)*

Boulder, CO

*Nathan Gonzalez (CTL):* Homodyne Tomography for Characterization of Non-classical Optical States in Quantum Networking

*Jessica Gerac (MML):* Reproducibility in 3D Photopolymer Printing

*Jake Shin (ITL):* High Resolution Light Scattering Measurements of Information Displays

*Grant Mondeel (PML):* A Real-Time Data Analysis GUI for Transition-Edge Sensor Array Spectrometers

*Jacob Stuligross (PML):* Software to Support Gamma-ray Spectrometry

*Ethan Sontarp (MML):* Molecular Dynamics Simulations of Aqueous NaF using Polarizable Force Fields

*Essa St George (CTL):* Laser Scanning Microscope for High-Speed Waveform Metrology

*Anh Katerine Le (PML):* Clock Data Analysis Using Least Squares and Allan Variance Techniques

*Adam Keim (CTL):* Cryogenic low-noise DC measurements of nanoscale Josephson junctions

*Tuan Anh Nguyen (PML):* Characterizing extended InGaAs photodiode shot noise at 4 K

*Matthew Rilloraza (PML):* Frequency Comb Calibrated Laser Heterodyne Radiometry for Precision GHG Measurement

*Anthony Adesso (PML):* Accessible smartphone-based pH sensors using magnetic hydrogels

*Victor Lita (CTL):* Optimizing Electrochemical Reactions for Microwave Microfluidic Analysis

*Kayla McCreary (MML):* Comparing THC Recovery from Impaction and Electrostatic Filter Devices

*Natalie Bruhwiler (PML):* Radio frequency induced heating of passive implants during low field MRI

*Kamakshi Subramanian (PML):* MRI of Tumor Mimics with Quantitative and Radiomic Analysis

*Ellen Meyer (PML):* Robotic Calibration for Scales Used to Measure Radiation Pressure

*Ernesto Flores (PML):* Measuring Metal-Melting Lasers at their Focus

*Eve Blank (ITL):* Pareto Tracing Ridge Profiles for Wind Turbine Design

# SURF Student Colloquium

NIST – Boulder, CO

August 1-3, 2023

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|---|---|
| **Name:** | Nathan R. Gonzalez |
| **Academic Institution:** | Gordon College (Wenham, MA) |
| **Major:** | Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Pursue a Ph.D. in Physics |
| **NIST Laboratory, Division, and Group:** | Communications Technology Laboratory, RF Technology Division, High Speed Waveform Metrology Group |
| **NIST Research Advisor:** | Dr. Tasshi Dennis |
| **Title of Talk:** | Homodyne Tomography for Characterization of Non-classical Optical States in Quantum Networking |

**Abstract:**

We implemented optical homodyne tomography to characterize non-classical states of light, with the aim of creating optical networking between superconducting quantum computers. Tomography uses repeated samples of a light field to reconstruct a statistical measurement of its quantum state. Accurate characterization of quantum states is essential to assess the quality of the generated network entanglement and its ability to overcome transmission loss. In this process we developed a Mach-Zehnder interferometer for initial testing, implemented balanced detection, characterized quantum noise, and technical sources of noise inherent in the experiment. We employed a balanced detection scheme to measure field quadratures to which we applied maximum likelihood estimation as a statistical method to represent the quantum state. Characterizing our sources of noise allowed us to have a fundamental understanding of how to reduce detection error. In this talk we will show experimental measurements of a coherent quantum state, indicative of a laser.

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| **Name:** Jessica Gerac | | |
| **Academic Institution:** Appalachian State University | **Major:** Physics | |
| **Academic Standing (Sept. 2023):** | Junior | |
| **Future Plans (School/Career):** | Graduate School | |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory, Applied Chemicals and Materials Division, Nanoscale Reliability Group | |
| **NIST Research Advisor:** | Dr. Jason Killgore | |
| **Title of Talk:** | Reproducibility in 3D Photopolymer Printing | |

**Abstract:**

Additive manufacturing is a growing field with wide-reaching applications in the fabrication of precision parts. Recent progress in the 3D printing industry has yielded increasingly impressive visual results, but current methods fall short on metrics of accuracy, precision and reproducibility. Digital Light Processing (DLP), a type of vat photopolymerization that works by curing an entire layer of a print at once, is no exception. Variables like light intensity, wavelength, exposure duration, and mask complexity all have substantial impacts on DLP print outcome, yet these effects remain poorly understood. We aim to advance scientific understanding of these effects by creating hundreds of test masks under varying conditions and analyzing the resulting structures. Many advanced applications of 3D printing, such as the printing of replacement organs, require extraordinary precision and consistency at the microscale. To assess whether the print process exhibits the necessary level of detail, we employ Laser Scanning Confocal Microscopy, a technique that allows us to measure print geometries with sub-micron precision. The results of this study will contribute to the development of more accurate and reliable fabrication techniques by helping identify the causes behind unwanted effects. Moreover, by finding conditions that optimize print reproducibility, we pave the way for cleaner input data for machine-learning and data-driven models of the printing process.

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|---|---|
| **Name:** Jake Shin | |
| **Academic Institution:** Princeton University | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Junior (Third Year) |
| **Future Plans (School/Career):** | Complete my undergraduate studies and pursue a graduate degree. |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Software and Systems Division |
| **NIST Research Advisor:** | Mentor: Dr. John Penczek<br>NIST Host: Dr. Bradley Alpert |
| **Title of Talk:** | High Resolution Light Scattering Measurements of Information Displays |


**Abstract:**

Light scattering measurements off surfaces have a broad range of applications, ranging from photorealistic rendering in computer graphics to modeling the surface roughness of materials. An important consequence of light scattering is its impact on the visibility of information, whether it be printed or electronic information. With rising consumer expectations, further development and optimization of information displays requires a concrete metric for characterizing light scattering.

One approach for quantifying these scattering properties is by measuring the Bidirectional Reflectance Distribution Function (BRDF) of a surface. This angular scanning measurement allows us to characterize the relationship between the incident and reflected light off of materials in terms of three empirical scattering attributes: Specular (mirror-like), Lambertian (perfectly diffuse), and Haze (directionally diffuse).

In this project, we built a 4-axis motion system to make in-plane BRDF measurements for a number of surface samples. We automated the angular scanning procedure by developing MATLAB user interface drivers for the apparatus. This automation enables us to conduct high resolution scans with a broadband white light source, in which the reflected light is collected via a photometric detector. The high resolution of these BRDF measurements then allows us to identify and extract the relevant empirical scattering attributes, which can provide a model to assess the performance and design of the sample.

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| **Name:** Grant Mondeel | | |
| **Academic Institution:** Clemson University | **Major:** Physics | |
| **Academic Standing (Sept. 2023):** | Junior | |
| **Future Plans (School/Career):** | Pursue a PhD in physics. Research at a national lab. | |
| **NIST Laboratory, Division, and Group:** | PML, Division 687, Quantum Sensors Group | |
| **NIST Research Advisor:** | Galen O'Neil | |
| **Title of Talk:** | A Real-Time Data Analysis GUI for Transition-Edge Sensor Array Spectrometers | |

**Abstract:**

Transition-edge sensor array (TES) spectrometers are used in many fields of physics to measure radiation with high precision and across a large bandwidth. For instance, TES spectrometers are used to probe extremely high electric field physics by observing x-ray transition lines from highly-charged ions from the NIST electron beam ion trap (EBIT) and from exotic atoms formed from a nucleus and a muon at the Japan Proton Accelerator Research Complex (JPARC). Despite the potential of TES spectrometers, analyzing the raw current timestreams to high resolution lists of time and energy for each photon arrival is still done with clunky software and is largely inaccessible to non-specialists. Here we describe a graphical user interface (GUI) which presents existing data analysis methods in a more intuitive and accessible format. This new format has also allowed for more thorough real-time analysis of data during experiments. Specifically, the GUI can be used to view spectra as data is being collected so that scientists can make informed decisions about how to allocate valuable experimental time. The same GUI can perform the final analysis of data that is amenable to standard processing methods. Streamlining TES data analysis puts the focus back on the physics being studied and will make future experiments more efficient.

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**Name:** Jacob Stuligross

**Academic Institution:** Vassar College | **Majors:** Physics, Mathematics

**Academic Standing (Sept 2023):** Recent graduate

**Future Plans (School/Career):** Automation and test engineer for a while, then physics graduate school

**NIST Laboratory, Division, and Group:** Physical Measurement Laboratory, Quantum Electromagnetics Division, Quantum Sensors Group

**NIST Research Advisor:** Daniel Becker

**Title of Talk:** Software to Support Gamma-ray Spectrometry

**Abstract:**

Materials accounting is a crucial part of nuclear safeguards. Measuring the isotopic composition of samples of actinides including Uranium and Plutonium are particularly important. Non-destructive analysis (NDA) relies on gamma-ray detectors and gamma spectrum analysis. The current state-of-the-art technology for NDA is high-purity Germanium (HPGe) detectors, which allow for Plutonium isotopic ratio uncertainties as low as 1 - 3 %. But in large nuclear facilities, even lower uncertainties are necessary which can only be achieved by destructive measurements like mass spectrometry. These measurements are slower, costlier and require materials handling.

Transition-edge sensor (TES) microcalorimeters are an emerging technology which utilize the high temperature sensitivity of superconductors near their transition temperature to make precise measurements of the energy of photons. The high temperature sensitivity provides energy resolution 10 times better than that of HPGe detectors, reducing the impact of systematic effects such as peak overlaps, and which should allow microcalorimeters to achieve uncertainties of less than 1 %. TES microcalorimeters thus provide potential for reducing reliance on destructive analysis in nuclear facilities. However, as a new technology, analysis software supporting the excellent energy resolution of microcalorimeters is currently immature.

This SURF project was dedicated to developing a user interface for an existing analysis code, SAPPY, and extending its capabilities. SAPPY was written in Python for Plutonium isotopic analysis on gamma-ray spectra from both HPGe detectors and TES microcalorimeters. The user interface was inspired by existing HPGe analysis tools like FRAM, which will help this new platform be adopted and used at other facilities for isotopic analysis from TES microcalorimeters.

Another part of this project is to use Monte Carlo simulations of TES microcalorimeter spectra to validate the performance of SAPPY's curve-fitting code. Asymmetric peaks in TES microcalorimeter spectra can arise from photons absorbed by a TES microcalorimeter before it has cooled off enough from the previous absorption. SAPPY fits peaks symmetrically, which may result in errors in estimates of peak areas and therefore isotopic ratios if asymmetric peaks are present.

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| **Name:** | Ethan Sontarp |
| **Academic Institution:** | Princeton University |
| **Major:** | Geosciences |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Pursue a Ph.D. in Geochemistry |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory, Applied Chemicals and Materials Division, Thermodynamics Research Center |
| **NIST Research Advisor:** | Dr. Demian Riccardi |
| **Title of Talk:** | Molecular Dynamics Simulations of Aqueous NaF using Polarizable Force Fields |


**Abstract:**

Alkali halide salts, such as NaF, serve as model systems for probing the solvation and association characteristics of ions in water. In solution, ions may exist in distinct association modes, such as unpaired free ions (FI), in singly or doubly solvent-separated ion pairs (SIP, DSIP), or as contact ion pairs (CIP). These association modes differ in their electrostatic interactions with water. Nuclear Magnetic Resonance (NMR) experiments conducted in the NIST Applied Chemicals and Materials Division have discerned a dependence of Na-23 and F-19 nuclei chemical shifts on temperature and solution concentration; extensive molecular dynamics (MD) simulations with fixed-charge force fields have been used to examine the molecular details of these experimental observations. Fixed-charge force fields are widely employed in the simulation of condensed-phase processes, however, the accuracy of MD simulations is dependent on the accuracy of the governing physical models and their parameterization. Ideally, ab initio MD may be applied to the study of aqueous systems, yet quantum mechanical methods remain computationally costly, restricting the duration and size of simulated systems. Polarizable force fields allow for improved accuracy of the physical models with reasonable computational efficiency on GPUs. We use the GPU-accelerated Tinker9 software to apply the AMOEBA09 polarizable force field to aqueous NaF, providing a means of comparison with previous fixed-charge force field simulations. We develop a streamlined workflow that uses PackMol to initialize the unit cell geometry, then Tinker9 programs for minimization, equilibration, and data production. The workflow is implemented in a Gitlab repository and has been deployed on several NIST GPU clusters. Structural analysis is carried out using the python package MDAnalysis. We characterize the effect of temperature on local hydration and the relative presence of FI, SIP, DSIP, and CIP associations. We show that the carefully parameterized, fixed-charge force field of Fyta and Netz (2012) is in reasonable agreement with AMOEBA09 for NaF, an observation unlikely to hold for larger, more polarizable ions.

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| **Name:** Essa St George | |
| **Academic Institution:** Bethel University | **Major:** Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Most likely pursue a career in industry for a few years before considering grad school |
| **NIST Laboratory, Division, and Group:** | Communications Technology Lab, RF Technology Division, High-speed Waveform Metrology Group |
| **NIST Research Advisor:** | Bryan Bosworth |
| **Title of Talk:** | Laser Scanning Microscope for High-Speed Waveform Metrology |


**Abstract:**

Wireless communication technology is increasingly moving toward the use of millimeter-waves with frequencies of 100 GHz and beyond. Optical sources such as ultrafast lasers conveniently offer several THz of available bandwidth for waveform generation and measurement in this range. Engineers are already developing new integrated circuits to meet these needs. However, even though the ability generate extremely precise and programmable high-frequency waveforms exist, the tools for measurement often lag far behind as electronic devices are limited to frequencies below 67 GHz. In order to optimize energy efficiency and stability of high-frequency circuits, it is necessary to characterize the nonlinear properties of these new devices. To do this, better measurement systems are needed.

In this project, we combine techniques for electro-optic imaging of millimeter-wave propagation with laser scanning microscopy. Using programmable spectral filters and state-of-the-art photodetectors, we can generate voltage waveforms on-wafer well beyond the limitations of electronic digital-to-analog converters. With the help of electro-optic substrates, we can then optically measure these signals on-wafer with time resolution that is orders of magnitude beyond electronic capabilities. Using an array of sampling points along a waveguide allows for high-frequency spatio-temporal measurements. This on-wafer network analysis functions for frequencies up to 800 GHz. This summer, updates are being made to the microscope system to simplify mode switching and automate the scanning process.

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| **Name:** | Anh Katherine Le | | |
| **Academic Institution:** | University of Maryland, College Park | **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Junior | | |
| **Future Plans (School/Career):** | UMD Combined BS/MS Program | | |
| **NIST Laboratory, Division, and Group:** | PML - Time and Frequency Division | | |
| **NIST Research Advisor:** | Judah Levine | | |
| **Title of Talk:** | Clock Data Analysis Using Least Squares and Allan Variance Techniques | | |

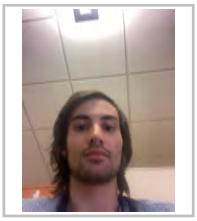
**Abstract**:

Clock data analysis plays a crucial role in many scientific disciplines, such as navigation systems, communication networks, and scientific experiments. I'll mainly discuss the application of two important techniques, namely least squares and Allan variance, for analyzing clock data.

The least squares method estimates and models clock behaviors. By minimizing the sum of squared residuals, it facilitates precise determination of clock parameters, including frequency offset, phase offset, and drift. This technique enables accurate calibration of clocks by identifying systematic errors and facilitating corrective measures. Its vital role in enhancing clock accuracy and stability is indispensable for maintaining precise timekeeping and synchronization across diverse applications.

Conversely, the Allan variance technique focuses on evaluating clock stability and noise characteristics of clocks over different time intervals. By quantifying fluctuations in clock frequency or phase, it reveals short-term and long-term variations, including random noise, frequency drift, and aging effects. This analysis aids in assessing clock performance, predicting timing accuracy, and optimizing clock designs. As a fundamental tool in time and frequency metrology, it enables the characterization and comparison of clock stability, thus contributing to the development of highly accurate timekeeping systems.

The integration of least squares and Allan variance techniques in clock data analysis provides valuable insights into clock behavior, enabling precise synchronization, reliable timing, and enhanced system performance across a range of applications.



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| **Name:** Adam Keim | | |
| **Academic Institution:** Colorado College | **Major:** Physics, Chemistry | |
| **Academic Standing (Sept. 2023):** | Senior | |
| **Future Plans (School/Career):** | Graduate School | |
| **NIST Laboratory, Division, and Group:** | CTL, RF Technology Division, Superconducting Electronics Group (672.06) | |
| **NIST Research Advisor:** | Pete Hopkins | |
| **Title of Talk:** | Cryogenic low-noise DC measurements of nanoscale Josephson junctions | |

**Abstract:**

Josephson Junctions (JJ's) are superconducting devices with many applications in precision electrical metrology; for example, over a quarter million JJs are used in the primary 10 VDC voltage standard. JJ's with a physical size on the order of 100 nm and critical currents less than 100 nA are used as the nonlinear elements in superconducting quantum bits (qubits) in prototype quantum computers. Characterization of the DC and microwave electrical properties of these JJs is crucial to understanding and simulating qubit operation and lifetime. DC measurements of very small currents and voltages are susceptible to a variety of types of intrinsic and extrinsic noise, with the ideal measurement limited by the noise of the JJ itself. With the goal of accurately measuring the critical current and sub-gap resistance of junctions near this noise level, we designed and built a measurement circuit that uses instrumentation amplifiers on a printed circuit board to achieve low noise figures. We show DC measurements of junctions at cryogenic temperatures for micrometer-size JJs at 4 K and 100 nm size JJs at < 0.1 K.

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| **Name:** | Tuan Anh Nguyen |
| **Academic Institution:** | Stanford University |
| **Major:** | Physics |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Earn a PhD in Physics and work as an experimental physicist |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Time & Frequency Division, Precision Photonics Synthesis Group |
| **NIST Research Advisor:** | Franklyn Quinlan |
| **Title of Talk:** | Characterizing extended InGaAs photodiode shot noise at 4 K |

**Abstract:**

In the generation of microwave signals via photodiodes, timing stability is fundamentally limited by the phase noise originating from shot noise. Previous work involving picosecond pulse detection demonstrated that shot noise correlations can lower the phase noise floor by orders of magnitude below traditional estimates of the fundamental limit. In this project, we aim to confirm previous observations of a lowered phase noise floor at 4 K for an extended InGaAs photodiode. To reach the shot noise limit, we employ cross correlation and take advantage of cross spectrum collapse to average out reference oscillator noise and thermal noise, respectively. Our initial measurements of phase noise on a 5GHz carrier did not demonstrate the lowered noise floor we measured with other photodiodes, possibly indicating something occurring beyond our models. Moving forward, we will cross-correlate a 1GHz carrier to explore the possibility of a carrier frequency dependence of our measurements. A confirmation of a lowered phase noise floor persisting at 4 K impacts a broad range of applications that rely on cold, stable microwave generation, a promising one involving scalable, superconducting quantum computers.

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| **Name:** Matthew Rilloraza | |
| **Academic Institution:** University of Illinois at Urbana-Champaign | **Major:** Engineering Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate School |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Time and Frequency Division, Precision Photonic Synthesis Group |
| **NIST Research Advisor:** | Dr. Ryan Cole |
| **Title of Talk:** | Frequency Comb Calibrated Laser Heterodyne Radiometry for Precision GHG Measurement |


**Abstract:**

The precision measurement of greenhouse gases remains a potent issue in the world of climate monitoring, flux estimations, and carbon budgeting. Next-generation GHG instrumentation would be required to have precision and accuracy on the order of ppb or better to match measurement recommendations given by climate agencies such as the World Meteorological Organization. Laser heterodyne radiometry (LHR) provides a relatively simple and inexpensive means to take total column measurements of trace atmospheric gases, and when coupled with laser frequency comb calibration, atmospheric absorption transitions can be measured to extremely high precision and accuracy.

My work this summer involved various aspects of this precision spectroscopy process. Frequency comb calibration ensures absolute frequency certainty, but in order to validate the absolute accuracy of the LHR system for GHG mixing ratio measurements, I created an optical setup with a 30 m Herriott gas cell which will be used for laboratory spectroscopy of known species concentration. Additionally, for solar absorption spectra measurement in the field, I improved upon multiple components of the data analysis process. I analyzed the signal-to-noise ratio (SNR) of measured spectra and compared these measurements to theoretical predictions. This comparison is of great importance for assessing overall instrument performance. In the computational realm, spectral line fitting becomes complicated by the fact that the atmosphere is not homogeneous but layered; thus, I explored computationally efficient methods for fitting the immense number of spectra recorded on a given day.

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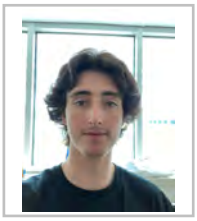
| **Name:** | Anthony Adesso | |
| **Academic Institution:** | Florida State University | **Major:** Chemical Engineering |
| **Academic Standing (Sept. 2023):** | Masters Student | |
| **Future Plans (School/Career):** | A Master's degree at FSU | |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Applied Physics Division, Magnetic Imaging Group | |
| **NIST Research Advisor:** | Gary Zabow/Mark Ferris | |
| **Title of Talk:** | Accessible smartphone-based pH sensors using magnetic hydrogels | |

**Abstract:**

Current pH sensor technology relies on the use of either expensive electronic pH meters, or cheap and inaccurate litmus paper strips. While the latter is quick and accessible to the general public, it relies on the use of color to determine the pH of the solution. This qualitative result prevents precise readings and poses challenges to users who may have color vision deficiency. The goal of this research is to develop a low-cost and quantitative alternative to these tests. This investigation uses a magnetic hydrogel strip that can interface with the magnetometer chip in any common smartphone. This strip is a bilayer consisting of an inert hydrogel layer and a thin, pH sensitive active layer. The active layer swells with an increasing pH, resulting in the strip curling away from the magnetometer in the phone. This mechanical change in structure results in a lower measured magnetic field reading, which can then be used to determine the pH of the test solution based on a prior calibration. The molar ratio of the backbone monomers and the solvent concentration in the active layer were tuned to control the initial curvature of the hydrogel strip, allowing the sensor to be "tuned" for desired initial pH values. Additionally, the maximum magnetic field strength was controlled by changing the magnetic particle loading within the active layer.



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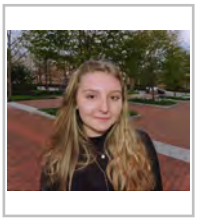
| **Name:** Victor Lita | | |
| **Academic Institution:** | Cal Poly San Luis Obispo | **Major:** Chemical Engineering |
| **Academic Standing (Sept. 2023):** | Upcoming Junior | |
| **Future Plans (School/Career):** | Undecided | |
| **NIST Laboratory, Division, and Group:** | CTL, RF Technology, Guided Wave Electromagnetics Group | |
| **NIST Research Advisor:** | Jacob Pawlik | |
| **Title of Talk:** | Optimizing Electrochemical Reactions for Microwave Microfluidic Analysis | |

**Abstract:**

Electrochemical synthesis has long been a common industrial technique to produce value-added chemicals at a large scale due to the low cost, simple reaction setup, and high selectivity of the process. However, the composition, kinetics, and mechanisms of most organic electrosynthesis reactions are still largely unknown. In order to characterize these reactions thoroughly, we must study their dynamics over a wide range of timescales. We will utilize microwave microfluidic spectroscopy to measure the broadband impedance of electrochemical reactions on a microfluidic chip and capture events with millisecond to picosecond timescales. We will measure spectra from 40 kHz - 110 GHz of a model reaction (Shono oxidation of N-Boc pyrrolidine) and correlate spectral features to specific electrochemical mechanisms. The collected impedance spectra will offer information on various phenomena including electrical double layer formation, ionic conductivity, and dipolar relaxations, which are directly associated with reaction yield and molecular properties. In order to prime the Shono oxidation reaction for measurement, we will determine ideal starting materials, concentrations, and electrical conditions with a conventional electrolysis setup. Electrolysis will be performed under either potentiostatic or galvanostatic conditions, and product formation will be confirmed through nuclear magnetic resonance spectroscopy. Once the product yield of the reaction is optimal, we will obtain microwave microfluidic spectra at different stages throughout the reaction process in order to characterize the electrical properties and composition at these different stages. Ultimately, our goal is to transfer our reaction to the microfluidic chip so that we can perform in situ measurements of the electrochemical system as the reaction is happening. We expect that our measurement technique will expand the frequency range of impedance spectroscopy into the GHz regime and uncover new insights into the mechanisms of electrically driven synthetic processes.



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**Name:** Kayla McCreary

**Academic Institution:** The Pennsylvania State University | **Major:** Chemistry

**Academic Standing (Sept. 2023):** Graduated in May 2023

**Future Plans (School/Career):** Ph.D. Chemist, Kansas State University

**NIST Laboratory, Division, and Group:** Materials Measurement Laboratory, Applied Chemicals and Materials Division, Fluids Characterization Group

**NIST Research Advisor:** Dr. Jennifer Berry


**Title of Talk:** Comparing THC Recovery from Impaction and Electrostatic Filter Devices


**Abstract:**

As cannabis legalization increases across the United States, impaired driving due to cannabis use is a growing concern. Currently, there are no established legal limits in blood or breath regarding delta-9-tetrahydrocannabinol (THC), the main psychoactive molecule in cannabis. While a cannabis breathalyzer that can be used similarly to an alcohol breathalyzer at roadside would be preferred, such a device does not exist for a variety of reasons. Ethanol is copiously present in breath as a vapor, but THC does not behave the same as ethanol. THC has very low volatility and has been theorized to be carried in breath aerosol particles formed from lung surfactant. Breath aerosols can be recovered on filter devices and THC has been detected after recent cannabis use with three different breath aerosol collection devices. As these studies are limited to small population sizes, more fundamental research needs to be done with these devices. An area of necessary research is establishing a percent recovery for these breath collection devices. This project establishes a THC recovery protocol for impaction filter devices for quantitative analysis first with an impaction filter device called Breath Explor. Filter devices were spiked with THC after being prepared with breath matrix. Ethylene glycol was utilized as a keeper in the elution solvent, which was vacuum concentrated and reconstituted. The breath samples were analyzed by liquid chromatography with tandem mass spectrometry (LC-MS/MS). Two initial studies show that the average THC percent recoveries from the Breath Explor devices were 14.8% and 21.1% on average. A similar elution protocol will be applied to the SensAbues device, which uses an electrostatic filter, so that THC recovery between devices can be compared.

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| **Name:** | Natalie Bruhwiler |
| **Academic Institution:** | University of California, Berkeley |
| **Major:** | Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate program |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Applied Physics Division, Magnetic Imaging Group |
| **NIST Research Advisor:** | Katy Keenan, Stephen Ogier |
| **Title of Talk:** | Radio frequency induced heating of passive implants during low field MRI |


**Abstract:**

Low-field MRI has recently sparked a lot of interest due to its accessibility and safety benefits, and there are new, FDA-approved systems available at field strengths between 64 mT and 0.55 T. Because of this, it would be useful to expand existing safety procedures to include low-field MRI.

One safety concern during MRI scans is radiofrequency-induced heating of passive implants. Passive implants are medical devices that do not require an external power source, for example stents, catheters, electric leads, and certain prostheses. During MRI, radiofrequency fields induce electrical eddy currents in these implants. This can cause localized heating on or near the implant, which poses a risk to the patient.

ASTM International (an international standards organization) has published a standard test method for measuring the heating of passive implants during MRI [1]. The method uses a gelled-saline that mimics the dielectric properties of human tissue. However, these properties change depending on frequency, and scanners with different magnetic field strengths operate at different frequencies. The mixture defined by ASTM International is valid at typical clinical magnetic fields (1.5 T and 3 T), but not at low fields.

This project involves developing several gelled-saline mixtures that mimic dielectric properties of human tissue at the frequencies used by low-field MRI. These mixtures will contain distilled water,sodium chloride, and polyacrylic acid (for gelling). We plan to embed an implant in the gelled-salines and measure the change in temperature on or near the implant using fiberoptic thermometers according to the ASTM International standard test method. These tissue mimic recipes can then be used by implant and scanner manufacturers to determine whether it is safe for someone with a passive implant to receive a low-field MRI scan.



[1] https://www.astm.org/f2182-19e02.html

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|---|---|
| **Name:** Kamakshi Subramanian | |
| **Academic Institution:** Wellesley College | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Graduate school in physics, biophysics, or biomedical engineering |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Applied Physics Division, Magnetic Imaging Group |
| **NIST Research Advisor:** | Stephen Russek |
| **Title of Talk:** | MRI of Tumor Mimics with Quantitative and Radiomic Analysis |

**Abstract:**

Quantitative MRI and radiomic analysis are valuable tools in medicine for the diagnosis and treatment of tumors in patients, particularly due to their ability to provide detailed information on tumor size, shape, and structure, as well as their underlying tissue structure and heterogeneity. The development of a tumor mimic, which is tailored to match human tissue and 3D printed based on quantitative MRI data from a real patient's tumor, would be of significant use to doctors as a medical standard. In this project, a 3D printing process, based on the FRESH printing process, was applied on a HyRel ESR printer to build these tumor mimics, using alginate gel as a support bath and various polymerizing chemicals as bio-inks and curing agents. The chemicals both crosslink with the alginate to create a solid 3D structure with defined shape and dimensions within the gel as well as alter the T1 and T2 values in the resulting section of the polymer. The 3D printed mimics were then placed in an MRI scanner and the resulting T1, T2, and diffusion maps were analyzed in different regions of interest to determine if the contrast agreed with the original image. A Python bioprinting program enabled rapid iteration of the process by downloading a DICOM image and converting the brightness values from the resulting array directly into movement and extrusion commands in Gcode for the printer to execute, allowing back-and-forth rastering in 1 mm voxels with a greater degree of accuracy. Various challenges related to the relative viscosities of the gel and bio-inks were addressed by adjusting the extrusion parameters of the printer and the temperature of the print bed. MRI data leading to the final choice of materials used to bioprint various specific parameters is discussed, obtained by syringing and imaging different combinations of chemicals along the way. Quantitative values measured at different stages in the material development process are also presented. Further extensions of this project include the use of other printing techniques, such as photopolymer printing, to achieve the desired MRI values in different layers of the tumor structure.

# SURF Student Colloquium

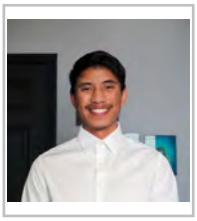
NIST – Boulder, CO

August 1-3, 2023

| | |
|---|---|
| **Name:** | Ellen Meyer |
| **Academic Institution:** | University of Rochester |
| **Major:** | Mechanical Engineering and Math |
| **Academic Standing (Sept. 2023):** | Fifth Year |
| **Future Plans (School/Career):** | Graduate School |
| **NIST Laboratory, Division, and Group:** | PML, Applied Physics Division, Sources and Detectors (686.01) |
| **NIST Research Advisor:** | Paul Williams |
| **Title of Talk:** | Robotic Calibration for Scales Used to Measure Radiation Pressure |

**Abstract:**

Radiation pressure power meters measure the optical power of a laser by measuring the force that a laser beam imparts when reflecting off a mirror. This force is typically measured by a sensitive balance that requires calibration from 100 μg to 100 mg. However, the masses used for this calibration are small and delicate, and a robotic system is required for placement of the masses. This project develops a three-axis robotic mass calibration system to place and remove masses from the balance and collect data from repeated measurements of multiple masses. This requires designing and 3D printing a mass "garage" to hold several masses and writing a LabView program that directs the robot to transfer each mass to the balance, use it to collect calibration data, and return it to the garage. The robotic calibration system helps to reduce noise in the calibration data by removing the human interaction. It also allows mass calibrations to be performed overnight when the environmental vibrations are less, and it makes it more convenient to collect a large number of measurements, which helps in statistical noise reduction. In this presentation I will discuss the field of radiation-pressure-based laser power measurements, the components of the robotic system, and the process of programing its movement.



# SURF Student Colloquium

NIST – Boulder, CO
August 1-3, 2023

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|---|---|---|
| **Name:** Ernesto Flores | | |
| **Academic Institution:** The University of Texas at San Antonio | **Major:** Physics | |
| **Academic Standing (Sept. 2023):** | Senior | |
| **Future Plans (School/Career):** | Graduate School in Physics | |
| **NIST Laboratory, Division, and Group:** | PML, Applied Physics Division, | |
| **NIST Research Advisor:** | Brian Simonds | |
| **Title of Talk:** | Measuring Metal-Melting Lasers at their Focus | |

**Abstract:**

High-power lasers allow industries to cut steel, weld cars and smartphones, and 3D print metal parts. These technologies rely on delivering focused laser light with intensities on the order of 1 MW/cm^2 and diameters of 100 micrometers. Accurate and precise measurements of the beam intensity play a key role in the efficacy of these technologies. Commercial devices exist to measure the beam profile and propagation under these conditions, however, industry engineers report significant discrepancies in their results. Currently, there is no NIST-traceability for high-irradiance beam profiles, let alone more advanced characterization metrics like the so-called M^2 measurement. To address this problem, we are developing a system to quantify the variability of commercial beam profile devices under conditions relevant to laser metal manufacturing. Then, this system will be used to provide traceability and absolute uncertainty of commercial systems in order to make these measurements more reliable and useful to industry. Our findings show that beam profile measurements have a high sensitivity to noise that greatly affects the beam diameters determined by an algorithm. We are currently working on improving the background sensitivity and quantifying any variables that affect our measurements.

# SURF Student Colloquium

NIST – Boulder, CO

August 1-3, 2023

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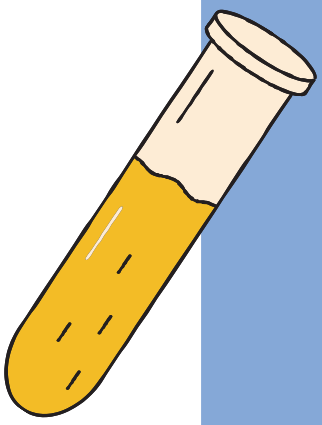
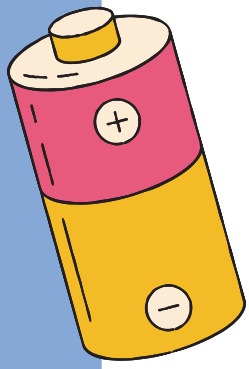
|---|---|
| **Name:** Eve Blank | |
| **Academic Institution:** Caltech | **Major:** Applied and computational mathematics |
| **Academic Standing (Sept. 2023):** | 4th year, GPA 3.6 |
| **Future Plans (School/Career):** | Undecided |
| **NIST Laboratory, Division, and Group:** | ITL 771-1 |
| **NIST Research Advisor:** | Zachary Grey |
| **Title of Talk:** | Pareto Tracing Ridge Profiles for Wind Turbine Design |

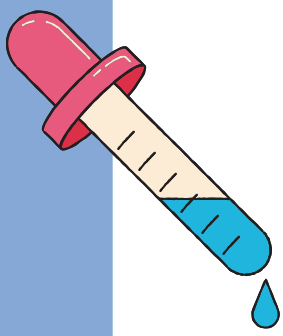
**Abstract:**

Pareto tracing defines the solution to bi-criteria optimization given as a path through parameter space which describes the optimal trade-off between two objectives. Directly computing the Pareto trace is often impossible over high dimensional parameter spaces since many applications---specifically wind turbine shape optimization---result in objective functions which do not vary over all parameter combinations. To address this impasse in wind turbine design, we explore the use of ridge approximations as surrogate functions to restrict the optimization over a data-driven subspace of reduced dimension to parametrize the trace. Additionally, we explore the concept of interpolating objective-dependent subspaces to define a variable subspace over the approximated trace. We apply this technique to approximate Pareto fronts describing optimal trade-offs between lift and drag forces induced over changing airfoil shapes used in wind turbine blade design.





NIST | COMMUNICATIONS TECHNOLOGY LABORATORY



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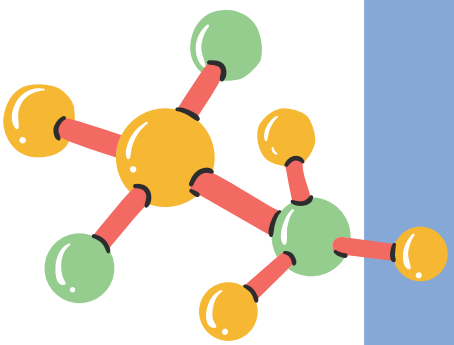


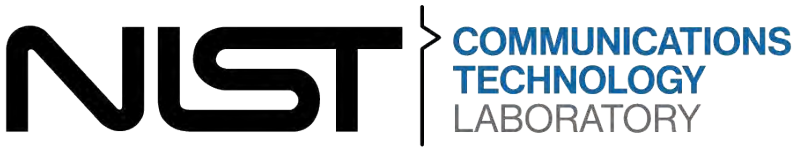
## Summer Undergraduate Research Fellowship (SURF) - 2023 Participants

*(in the order of the Colloquium schedule)*

Communications Technology Laboratory (CTL)

*Benjamin Philipose (virtual)*: Integrating Network Simulations for Enhanced Vehicle Performance Analysis

*Benjamin Winig:* Simulating Manufacturing Environments with SimPROCESD



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Benjamin Philipose |
| **Academic Institution:** | Seattle University |
| **Major:** | Computer Engineering/Computer Science |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Pursue Masters in Computer Science |
| **NIST Laboratory, Division, and Group:** | Communications Technology Labratory (CTL) |
| **NIST Research Advisor:** | Dr. Thomas Roth |
| **Title of Talk:** | Integrating Network Simulations for Enhanced Vehicle Performance Analysis |


**Abstract:**

Automated vehicles are becoming more prominent, and a potential feature of these cars is the ability to communicate with surrounding vehicles and infrastructure for better control. This communication must consider the physical constraints of the system, such as the weight of the car, or its grip on the road, which affect control decisions such as the amount of distance the car needs to safely brake. The timeliness of the information communicated is crucial as it allows vehicles adequate time to respond physically. Currently network simulators, such as ns-3 are used to provide insights into information arrival time and its impact, However, most approaches to date have focused mainly on network performance without realistic physics models that consider the vehicles dynamics. One approach to address this disparity, is to have ns-3 be able to communicate externally and co-simulate with an external physics simulator to provide insight on real time constrains. A challenge present with co-simulation is delays that can be introduced from transferring data between two simulations, which in a network simulation (ns-3) that focuses on timing, would not be ideal. Therefore, a gateway module is developed for the purpose of data transfer between ns-3 and external simulators, with a focus on maintaining low latency induced by its implementation. The primary objective of this research is to develop a simulation environment that accurately measures the impact of communication on automated vehicle performance. The approach is demonstrated through a braking scenario that involves three cars in a single lane. The gateway module, which acts as a bridge between ns-3 and a dynamic vehicle simulator, is implemented inside of ns-3 as a new module in C++. The lead car is scripted to stop at some point in the simulation, and it informs the other vehicles through vehicle-to-vehicle communication. By having the gateway module enable efficient data transfer between ns-3 and CARLA, the currently used dynamic vehicle simulator, the performance impact on vehicles can be measured based on realistic communication scenarios.

# SURF Student Colloquium

NIST – Gaithersburg, MD
August 1-3, 2023

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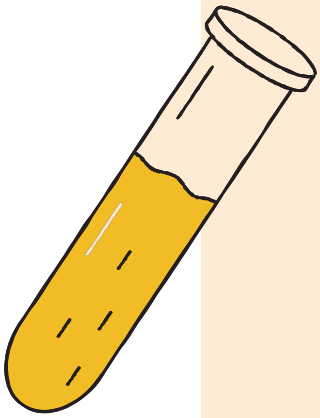
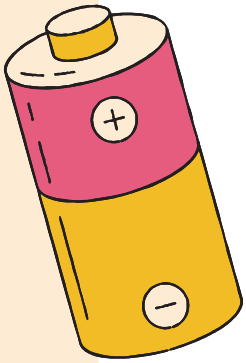
|---|---|
| **Name:** Benjamin Winig | |
| **Academic Institution:** University of Maryland | **Major:** Aerospace Engineering |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Software Engineer |
| **NIST Laboratory, Division, and Group:** | CTL, Smart Connected Systems Division, Industrial Artificial Intelligence Management |
| **NIST Research Advisor:** | Dr. Michael Sharp |
| **Title of Talk:** | Simulating Manufacturing Environments with SimPROCESD |

**Abstract:**

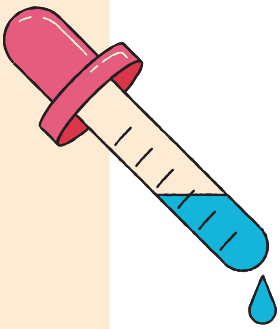
During production planning, manufacturers may consider different configurations of factory floor machinery and maintenance policies, especially policies enabled by the increasing availability of AI-based condition monitoring systems. Different machine configurations and maintenance policies have a profound impact on production performance. Insights on production-level impacts can be valuable during production planning. SimPROCESD (Simulated-Production Resource for Operations & Conditions Evaluations to Support Decision-Making) is an open-source simulation tool developed by NIST researchers that, with just a few lines of code, can quickly model and simulate the operations of a complex production system. This tool yields data that enables companies to quickly evaluate the effectiveness of maintenance policies and machine configurations regarding productivity, production quality, and reliability.

This talk will open with a summary of SimPROCESD and examples of how it applies to modeling manufacturing environments. The talk will then discuss event graphs we created to visualize and communicate the discrete-event simulation behaviors of SimPROCESD object models. This discussion will also showcase the extensibility of SimPROCESD to model object user-specific features. We then demonstrate the versatility of SimPROCESD by modeling a collaborative robotics example and analyzing its productivity and reliability.





NIST | DIVERSITY, EQUITY, & INCLUSIVITY OFFICE (DEIO)



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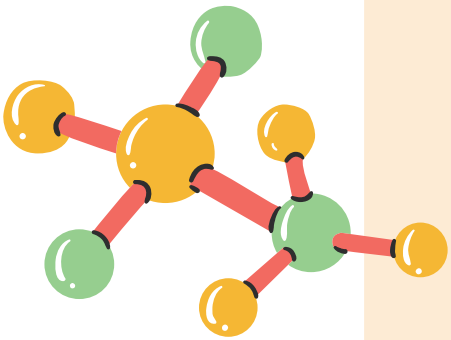

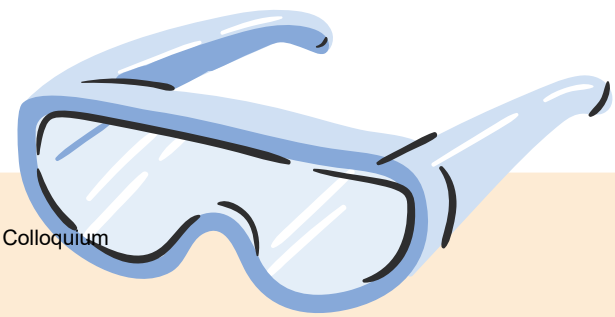

**Summer Undergraduate Research Fellowship (SURF) - 2023 Participants**

Diversity, Equity, and Inclusivity Office (DEIO)

*Ayomide Johnson:* Beyond words: Examining Implicit Social Expectations in Job Descriptions for Computer and Information Science Positions

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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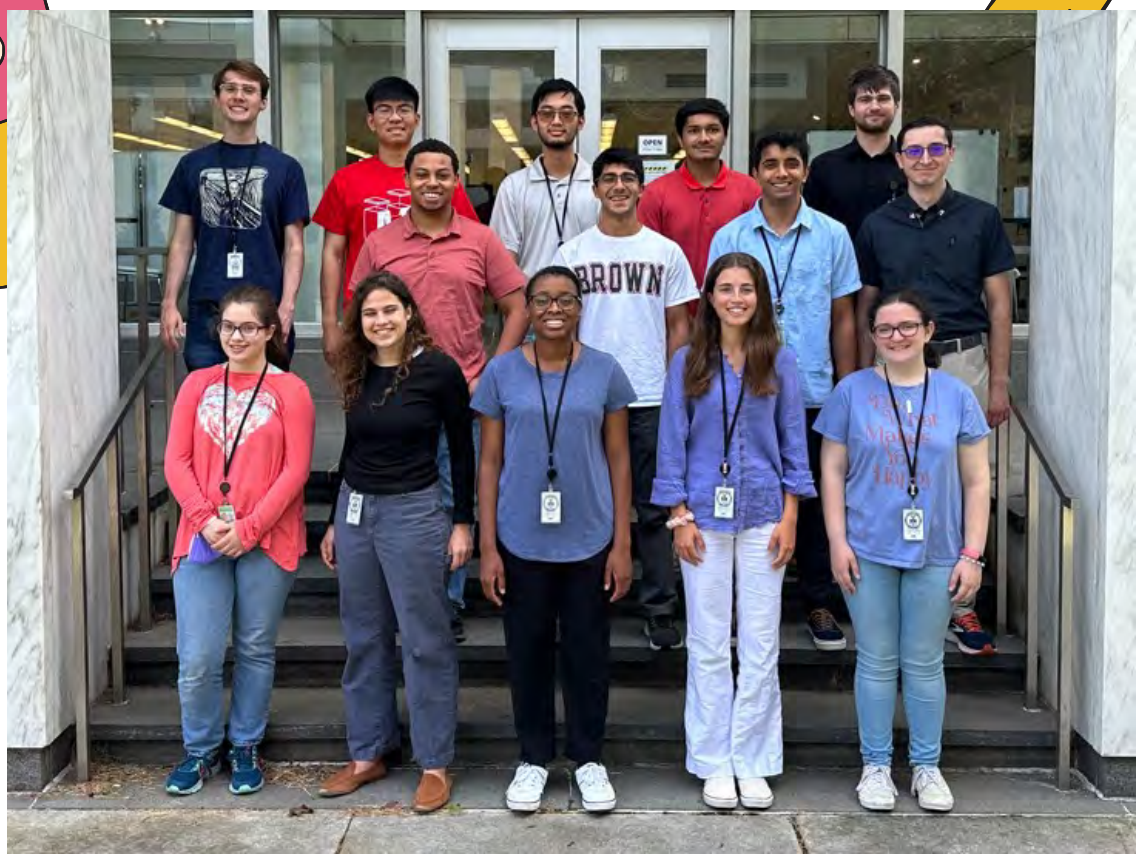
|---|---|
| **Name:** | Ayomide Johnson |
| **Academic Institution:** | Towson University |
| **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Rising Junior |
| **Future Plans (School/Career):** | I want to complete my undergraduate degree and later futher my education by aquiring my master's degree |
| **NIST Laboratory, Division, and Group:** | DEIO |
| **NIST Research Advisor:** | Jo Wu and Juan Fung |
| **Title of Talk:** | Beyond words: Examining implicit social expectations in job descriptions for Computer and Information Science positions |

**Abstract:**

Considering implicit biases in job descriptions for computer and information science positions is crucial if we hope to encourage diversity, ensure ethical hiring practices, and tackle bias in hiring process. Through the identification and challenging of implicit expectations in job postings, we can eliminate barriers to recruitment that disproportionately affect certain groups, and promote a more level playing field where everyone has equal opportunities. This will harness diverse experiences and perspectives that can drive innovation and creativity and ultimately lead to a better understanding of diverse user needs. Overall, assessing job descriptions for implicit biases is a key building block in creating more diverse, innovative, and ethical environments for the federal workforce.

The goal of this project is to investigate occupational segregation resulting from conscious and unconscious biases in the expectations of hiring managers. The first step in this research project is to investigate and curate a data set of historical job advertisements using the USAJOBS application programming interface (API) to compile roles and desired qualification descriptions. The text data and text mining methods are used to look for indicators of employer or recruiter bias in Computer Science occupational series. The project documentation provides the rationale behind the approach in the engineering decisions throughout the code development and curating of the data set. This makes the process more transparent and reproducible. This approach can also be scaled up to investigate API data in industries or institutions where occupational composition or demographic concentration distributions are incongruent with equitable access to occupational opportunity or economic security.




# Engineering Laboratory 2023

**Summer Undergraduate Research Fellowship (SURF) - 2023 Participants**

*(in the order of the Colloquium schedule)*

Engineering Laboratory (EL)

*Anabel Kadri:* Degradation Mechanism and Failure Mode of Polymeric Backsheets used in Photovoltaics

*Rohan Hadavale:* Risk and Uncertainty in Community Resilience Planning

*Kristin Dan (virtual):* Determining a Built Infrastructure Vulnerability Index

*Hayley Pinkowitz:* Improving Technical Communications for the Engineering Laboratory

*Dhruv Rajagopal:* Using Comsol to Simulate Viscoelastic Fluid Motion Between Two Plates

*Janelle Davis:* Study of Pyrrhotite Reactions In Concrete

*Caden Williams:* Microscopy and Water-to  Cement Ratio of Concrete

*Samuel Chen:* Early Strength Development of Quick Setting Cement Mixtures

*Katherine Biernacki:* Exploring the Effect of Polyethylene Terephthalate Replacements in Portland Cement Mixtures

*Matthew Kubas:* Validation of the Reciprocity Law in the NIST 6-Port SPHERE Using Polyethylene Terephthalate

*Leon Zhang:* A Review of Public Radio Usage for Risk, Crisis, and Disaster Communication

*Eric Fagan (virtual):* Development and Utilization of a Database on Nonstructural Component Damage

*Varadraj Chavan:* Breaking Down Plastics: Unveiling the Degradation Process

*Braedon Mullin:* In-Situ Calibration of Differential Pressure Transducers

*Bradley Estacio (virtual):* Efficient and Compliance Check of HVAC information for Two NIST Facilities

*Robert Carlyon:* Predicting Wildfire Spread using Computational Fluid Dynamics

*Jaskaran Gill:* Online Documentation for NIST Fire Dynamics Simulator (FDS)

*Tiller Van Doren:* Fire Research Problem: Construction of Flame Spread Apparatus

*Nicholas Redford:* Interpolation of Flammability Behaviors through Different Materials

*Yehoshua Halle: Digital Twin Development for an Automated Robot Workcell*

*Ivon Charlery:* Digital Twin of Desktop Computerized Numerical Control Machine

*William Stiller:* Hierarchical Data Structure Development to Support Digital Thread and Digital Twin Applications

*Vladimir Alvarado:* Using Large Language Models to Help Formulate Scheduling Problems

*Tali Schlenoff:* InterFace the Facts

*Parker Liposky:* Aerial Drop Test Research

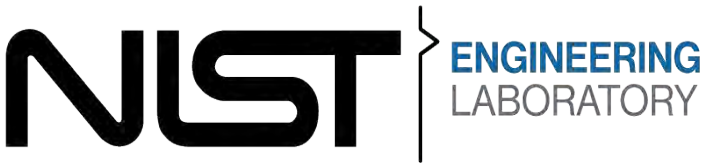
*Ethan Sundel:* Standardized Testing and Validation of Emergency Response Systems

*Brian Maloney:* ROS Integration with Agile Performance Robotic Systems

*Khoa Nguyen:* Collection, Analyzation, and Vizualizing of RGB and Depth Data for Human Study

*Noam Peled:* Real-time Pose Measurement to Support Robot Inspection

*Elijah Martin:* Developing a Custom Spin Coater Using a Microcontroller and 3D Printing



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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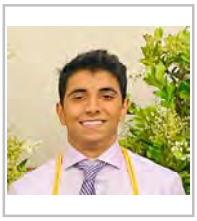
| **Name:** | Anabel Kadri | | |
| **Academic Institution:** | Tulane University | **Major:** | Enviornmental Earth Science |
| **Academic Standing (Sept. 2023):** | Junior | | |
| **Future Plans (School/Career):** | Attend graduate school | | |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Materials and Structural Systems Division, Infrastructure Materials Group | | |
| **NIST Research Advisor:** | Xiaohong Gu | | |
| **Title of Talk:** | Degradation Mechanism and Failure Mode of Polymeric Backsheets used in Photovoltaics | | |


**Abstract:**

Photovoltaic (PV) module polymeric backsheets provide electrical insulation and protection from environmental stressors, thus the performance of the backsheet directly impacts the operational lifetime of the PV module. The long-term reliability of PV modules is imperative as goals towards increased solar energy use are made. Backsheet defects are one of the most common causes of PV module failure, so understanding the degradation mechanism and failure modes of these components is critical to extending the lifetime and improving the efficiency of PV modules. The most common degradation factors are solar radiation, temperature, and moisture. When exposed to a combination of these factors, the backsheets can delaminate, discolor and crack, resulting in reduced power output or failure of the module altogether. New polymeric materials are being formulated in response to continued pressure to increase backsheet reliability and lower costs.

In this study, the durability of three different emerging polymeric PV backsheets was investigated. The polymeric backsheet films weathered in accelerated laboratory conditions were analyzed to study the aging behavior of the films. The samples were exposed to UV radiation under elevated temperatures and humidity using the NIST accelerated weathering device, i.e., the NIST Stimulated Photodegradation via High Energy Radiant Emission (SPHERE) device. Every 10 days the samples were analyzed for chemical, mechanical and optical changes. Characterization techniques included Fourier-transform infrared spectroscopy (ATR-FTIR), UV-Visible spectroscopy, and glossimetry and colorimetry. ATR-FTIR and UV-Visible spectroscopy measured chemical changes in the samples and glossimetry and colorimetry measured any optical changes such as discoloration. The data collected was used to better understand the degradation and failure modes of polymeric backsheets and provide insight into material selection and product development.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Rohan Hadavale |
| **Academic Institution:** | Irvine Valley College |
| **Major:** | Computer Science & Economics |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Transfer to a 4-year institution to complete undergraduate degree. Pursue a further education through an MBA program. |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, 730, Applied Economics Office |
| **NIST Research Advisor:** | Dr. Christina Gore |
| **Title of Talk:** | Risk and Uncertainty in Community Resilience Planning |


**Abstract:**

Community resilience is the ability of a community to prepare, protect, and recover in response to adverse situations such as disasters. When planning for community resilience, evaluating risk is an important factor when it comes to evaluate the allocation of community resources. However, it can be difficult to define risk because its meaning can vary across different disciplines. Whether it is economics, engineering, psychology, or some other field of study, each one tends to adopt its own unique terminology and framework to define and assess risk and risk preferences. Therefore, we must develop an interdisciplinary definition of risk in order to foster collaboration in research among various fields. First, we identified over 2,000 articles in the community resilience planning space using a keyword search. Those papers were then analyzed using a bibliometric analysis, which resulted in three distinct risk-based domains containing 141 papers. After aggregating the articles in the three main categories for mentions of risk, we utilized a text analysis tool and examine the displayed the bigrams and trigrams of the words that occurred most frequently within the text. The results showed that risk was being commonly used in different contexts across each of the three categories; one mentioned mostly risk perception, the other mentioned mainly risk assessment, and the third mentioned primarily risk communication. Based on the findings, the evident use of the word risk in various contexts shows the word s multifaceted nature within community resilience planning and creates a foundation to establish a comprehensive and interdisciplinary definition of risk.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Kristin Dan | |
| **Academic Institution:** University of Maryland College Park | **Major:** Applied Mathematics |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Career in data analysis and pursuing a graduate degree |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Applied Economics Office |
| **NIST Research Advisor:** | Dr. Jennifer Helgeson |
| **Title of Talk:** | Determining a Built Infrastructure Vulnerability Index |


**Abstract:**

Vulnerability is the relative measurement of the susceptibility of a community to be harmed by a shock or stress. Recent studies tend to focus on social factors when calculating vulnerability. However, models calculating vulnerability using social factors overlook the vulnerability of the built environment where the population operates.

The Built Infrastructure Vulnerability Index (BIVI) was created using factors associated with the built environment at the county level. These factors included variables such as number of business establishments, structure age, railroad track mileage, and broadband access. Using open-source data, many different variables relating to the built environment were collected. A principal component analysis with a varimax rotation was used to determine which variables were the most significant factors to create the BIVI score. Comparing heat maps of the BIVI, the Social Vulnerability Index (SoVI), and Community Resilience Estimates (CRE), will illustrate the relationship between social vulnerability and the built environment, as well as the contributing drivers. For example, a community may seem socially vulnerable, but a strong built environment may counteract a weak social environment, leading to less stress from hazards. An area's relative vulnerability is also dependent on the likelihood of a shock or stress affecting the area. Therefore, a scaled Hazard Score was created to illustrate areas that are both vulnerable and tend to experience a hazard occurrence.

Because of the wide range of variables the BIVI considers, the BIVI can help identify at-risk areas within the United States. Using social and built indices and examining the historical propensity for hazards is beneficial to recognizing factors contributing to an area's vulnerability. By identifying these factors, resources can be allotted to limit the risk corresponding to these factors.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Hayley Pinkowitz |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Mathematics and Economics |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | I plan to attend graduate school in economics |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory - HQ |
| **NIST Research Advisor:** | Kirk Dohne |
| **Title of Talk:** | Improving Technical Communications for the Engineering Laboratory |


**Abstract:**

Researchers in the NIST Engineering Laboratory (EL) do amazing work within their fields and communicate well with other researchers in their field through channels such as technical publications and conferences. However, they are not as adept at communicating their scientific findings with stakeholders and broader audiences in other scientific fields (including across NIST), the general public, and those in educational settings. To address this, I have created an Engineering Laboratory Communications Plan to help researchers understand the best communications channels to connect with different audiences and to illustrate best practices for using a selection of these communications channels. Having this guidance enables researchers to increase the impact of their work.

I focused on two areas within the EL Communications Plan for additional depth. The first, social media, is an area of weakness that can help individual researchers create a positive reputation and build an audience, while increasing the impact of their NIST research. Within the Plan, the social media section contains guidance on effective use and etiquette. Social media is an important path for EL to tell people what we *have done*. The second area of focus was the EL webpages for facilities. These pages provide insight into the Lab's scientific research capabilities and resources, information that illustrates what EL *can do*. I revised the template EL uses for these pages and updated/revised several of the facilities pages to make the information more easily understandable to multiple different audiences, including those not well-versed in scientific knowledge.

NIST EL communications is the last critical step to maximizing the impact of the amazing research done.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Dhruv Rajagopal |
| **Academic Institution:** | University of Illinois at Urbana-Champaign |
| **Major:** | Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Industry |
| **NIST Laboratory, Division, and Group:** | Engineering Lab, Materials and Structural Systems Division, Group 731 |
| **NIST Research Advisor:** | Dr. Nicos Martys |
| **Title of Talk:** | Using Comsol to Simulate Viscoelastic Fluid Motion Between Two Plates |

**Abstract:**

Understanding the rheological properties of cement paste is crucial in advancing and improving the process of cement 3D printing. As cement paste is a viscoelastic fluid, equations used in other viscoelastic experiments can be applied and adapted here. Comsol, a material simulation program, is used as a representation of the fluids being used, and the fluid properties and constituent equations can be edited to fit the needs of the experiment. This simulation focuses on the movement and behavior of a viscoelastic fluid between two parallel plates, with the top plate oscillating back and forth to create a shear force. In mathematical predictions and experimental trials of this behavior, a specific shape was found to be representative of the fluid on a stress-strain graph as well as a stress-shear rate graph. The purpose of the simulation is to be another comparison to the experimental model, and to be an easy way to predict the behavior of future trials for fluids with differing properties. Additionally, a model for the overall cement 3D printing process is being developed, including the flow through a pipe, deposition, and deformation over time, though this is less of a focus currently.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|
| **Name:** Janelle Davis | | |
| **Academic Institution:** | Northern Virginia Community College | **Major:** Engineering |
| **Academic Standing (Sept. 2023):** | Junior | |
| **Future Plans (School/Career):** | Aerospace Engineering B.S from Virginia Tech | |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Div. 731, Infrastructure Materials Group | |
| **NIST Research Advisor:** | Dr. Stephanie S. Watson | |
| **Title of Talk:** | Study of Pyrrhotite Reactions In Concrete | |


**Abstract:**

The degradation of concrete foundations is a rampant issue in various Connecticut structures. The presence of pyrrhotite in the concrete aggregate is the source of damage. This iron sulfide mineral undergoes oxidation reactions when exposed to moisture and oxygen. When pyrrhotite reacts, secondary products are formed which continue to compromise the structural integrity of concrete. Particularly, sulfate species attack the surrounding cement resulting in expansion and cracking. Concrete degradation presents high risks to safety and has severe economic implications. Generally, total foundation replacement is necessary to sufficiently resolve the problem. Currently, a standardized method to evaluate pyrrhotite quantities in aggregate and concrete is nonexistent. Therefore, the Infrastructure Materials Group (IMG) created reference materials (RM) that can be used with a variety of sulfur quantification test methods. IMG then developed a standard test method using x-ray fluorescence (XRF) to quantify sulfur species. This method uses ground cementitious materials specimens in a pellet form to preserve the initial sulfur species. The specimens are then reacted with borate reagents to oxidize all sulfur species to sulfate into a glass bead, which then provides a total sulfur concentration for each specimen. IMG has been working to develop calibration curves for this XRF test method and used the pyrrhotite RMs to generate specimens with varying pyrrhotite concentrations using a mix design. In this SURF project, a standard addition method is used to examine specific changes with sulfur concentration and XRF sulfur intensity. The total sulfur (S) content, including (0.5, 1 and 3) weight % of S, were prepared. Glass bead specimens were made with pyrrhotite, pyrite and gypsum, respectively, in a RM matrix. Stoichiometric calculations were performed to determine exact masses of each compound. The expectation is regardless of the type of sulfur compound used, each specimen should possess the same intensity as sulfur weight percentages are assumed to be "identical". The XRF instrument is used to measure the emission at the sulfur K alpha and K beta levels. The former level produces one peak and the latter can produce two peaks, which depends on the sulfur species. The original data output from the XRF program is reformatted into a traditional x (theta) & y (intensity) column table. To accomplish this efficiently, a python script was created to reorganize the data. The script was modified and reinterpreted to improve it. This XRF data, peaks and their intensity, is used to provide the sulfur concentrations from particular compounds. Upon analyzing the XRF data and confirming the intensities, calibration curves will be generated and the results from the various sulfur compounds discussed.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Caden Williams | |
| **Academic Institution:** Andrews University | **Major:** Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Get Professional Engineers license or sigma six, possibly grad school |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, 731, Infrastructure Materials Group |
| **NIST Research Advisor:** | Cody Strack |
| **Title of Talk:** | Microscopy and Water-to-Cement Ratio of Concrete |

**Abstract:**

The water-to-cement (w/cm) ratio is one of the most crucial properties of concrete, as it is connected to the strength of the concrete. A typical w/cm for a concrete mixture range is between 0.4 - 0.6, with the lower ratio typically indicating a higher strength of concrete, while the opposite is true for a higher ratio. Scanning electron microscopy was used to collect images of the sample using backscattered electrons, which caused contrast within the images. This contrast is then used, as elements lower on the periodic table will absorb more backscattered electrons and appear darker than elements of higher atomic numbers. This was used in conjunction with energy dispersive spectroscopy, which determined the chemical properties of the sample and aided in phase identification. Image analysis was conducted on the dataset using ImageJ, an open-source photo editing software, that enabled separation of the aggregate and cement phases in order to calculate the approximate w/cm of the different sections of the sample. By gathering enough images and collecting w/cm values, a general w/cm for the entire sample was calculated, giving insight into the concrete's strength.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Samuel Chen | |
| **Academic Institution:** University of Maryland - College Park | **Major:** Materials Science and Engineering |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Graduate School (currently undecided), Developing Green Technologies |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Materials and Structural Systems Division, Infrastructure Materials Group |
| **NIST Research Advisor:** | Dr. Aron Newman |
| **Title of Talk:** | Early Strength Development of Quick Setting Cement Mixtures |

**Abstract:**

Additive manufacturing of concrete, 3D printing using concrete extrusion, for residential homes is now available commercially and promises a reduced total resource costs as well as its ability to create structures otherwise impossible with conventional concrete placement that includes form work and pouring of concrete. The development of this technology has necessarily lead to the development of cement binders capable of setting in a much shorter timeframe so as to make the printing process possible in the first place. However, it remains unknown how exactly this change in binder composition impacts the mechanical properties of the resultant materials. As such, this study aims to address this gap in knowledge by synthesizing a popular quick-setting mortar blend and then determining its mechanical properties via micro-indentation which are cross-validated with bulk mechanical testing. The specific composition will be compared with a more typical mortar blend composed from ordinary Portland cement. A particular emphasis will be placed on measuring the early strength development of the tested blends, namely the strength of the mortars within a period of 1 day of setting. Little work has been done in this area in previous work as the knowledge of early strength development is simply unnecessary in conventional cast work. However, this knowledge is crucial to the further development of concrete additive manufacturing as it determines whether or not printed structures will collapse under their own weight with the addition of more printed layers.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Katherine Biernacki |
| **Academic Institution:** | Missouri University of Science and Technology |
| **Major:** | Ceramic engineering |
| **Academic Standing (Sept. 2023):** | Graduate student |
| **Future Plans (School/Career):** | Masters in Material engineering with thesis |
| **NIST Laboratory, Division, and Group:** | Engineering Lab, Materials & Structural Systems, Infrastructure Materials Group (731.07 Group 7) |
| **NIST Research Advisor:** | Rachel Cook, PhD |
| **Title of Talk:** | Exploring the Effect of Polyethylene Terephthalate Replacements in Portland Cement Mixtures |


**Abstract:**

Ordinary Portland cement (OPC) production is the source of 9–10% of anthropogenic carbon dioxide ($CO_2$) emissions. Thus, infrastructure material scientists have long pursued solutions to minimize OPC content in commercial building material mixtures in pursuit of eco-friendly material solutions. Plastics pose similar challenges. Globally, polyethylene terephthalate (PET) is one of the most utilized plastics for single-use applications. In 2015, the EPA reported that only 9.1% of the US's plastic waste gets recycled, and the rest is burned (15.5%) or, more commonly, landfilled (75.4%). Each landfilled piece of plastic degrades only after hundreds of years. Effective utilization of post-consumer waste plastic as a replacement material in OPC-based mixtures for construction applications could be an eco-friendly solution to both anthropogenic challenges. Physical techniques used include isothermal calorimetry and x-ray diffraction (XRD). The results show that alkaline solutions, such as pore solutions and OPC, promoted hydrolysis of the PET. Additionally, larger mass replacements of PET gave higher cumulatively released heat values compared to the 0% PET controls. At 72 hours, the heat released values are indicative of the progress of the overall reaction. When comparing the cumulative heat released per gram of OPC of the high replacement system to the control system on average, there is a 120% increase, that is, 544 J/g vs. 248 J/g.

This project seeks to explore the feasibility of using less cement while also encapsulating PET in cementitious mixtures. If successful, [OPC and post-consumer plastic] blends could be a feasible solution to limit the anthropogenic $CO_2$ footprint associated with OPC production and lessen the ever-growing plastic tide.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Matthew G. Kubas

**Academic Institution:** Illinois Wesleyan University | **Major:** Physics


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| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Washington University in St. Louis for a Second Bachelors in Electrical Engineering |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Materials and Structural System Division, Infrastructure Materials Group |
| **NIST Research Advisor:** | Deborah Jacobs |
| **Title of Talk:** | Validation of the Reciprocity Law in the NIST 6-Port SPHERE Using Polyethylene Terephthalate |


**Abstract:**

Laboratory accelerated weathering devices have been used to provide a means of predicting the service life of materials much faster than outdoor testing. Materials experience chemical and physical changes due to high intensity ultraviolet (UV) light in accelerated weathering settings compared to outdoor natural exposure. Temperature and humidity can also be controlled and repeated in these devices as opposed to natural weathering.

NIST Simulated Photodegradation via High-Energy Radiant Exposure (SPHERE) ensures even distribution of light using integrating sphere technology and controls temperature and relative humidity for 32 independently controlled sample chambers for accurate and reproducible results. It has been shown that the 2m SPHERE is able to degrade samples following the same mechanism naturally occurring with exposure to the outdoors. The original SPHERE has a 2-meter integrating sphere, with current development of a smaller, more intense 0.5-meter model, known as the 6-port SPHERE.

In this study, samples of polyethylene terephthalate (PET) were exposed to the 6-port SPHERE at different intensities using neutral density filters. These samples were intermittently tested for chemical changes using Fourier transform infrared spectroscopy (FTIR) and ultraviolet-visible spectroscopy (UV-Vis), measuring in the infrared and ultraviolet/visible regions, respectively. The results were compiled to show changes in the yellowing index and chemical properties of the exposed PET at specific wavelengths. These results were compared to previously collected results to establish the validity of the 6-port SPHERE. The higher intensity of the 6-port SPHERE will require future work encompassing the effect of low wavelength light with the use of cut-off filters at 295 nm, 305 nm, and 320 nm.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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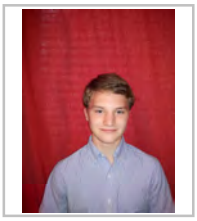
|---|---|
| **Name:** Leon Zhang | |
| **Academic Institution:** University of Maryland | **Major:** General Biology |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | MD and a career in Psychiatry or Internal Medicine |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Social Science Data Collection Considerations During Disaster |
| **NIST Research Advisor:** | Dr. Emina Herovic |
| **Title of Talk:** | A Review of Public Radio Usage for Risk, Crisis, and Disaster Communication |

**Abstract:**

Amateur 'Ham' Radio is one of the most reliable and accessible forms of sharing information for disaster communication (Ben-Enukora, Oyero, Okorie, 2014). While other communication mediums, such as internet or SMS, become unavailable during destructive events, radio's infrastructure allows it to be easier to access during disasters (Hugelius, Gifford, Ortenwall, 2016). Currently, minimal guidance exists for how to best use this medium for effective and life-saving communication during risk, crisis, and disaster. A systematic literature review on public radio for risk, crisis, and disaster communication was conducted to understand the state of knowledge on this topic and outline areas for future research exploration for both receivers and communicators of radio communication. Literature was gathered through an exhaustive search of online research databases and government websites and carefully reviewed for relevance, yielding 23 articles. Findings from prior studies suggest a gap in public knowledge and usage of Amateur Ham Radio for disaster preparedness and a potential lack of public awareness of how to receive important emergency information. Findings from extant literature also suggest that minimal guidance exists for communication best practices or standards via radio. Existing guidance suggests providing accurate, timely, well distributed, and easily accessible information, however further breadth and depth of guidance across various scenarios and applications may help to improve communication via this forgotten, but important medium. The common stance that almost all literature on radio communication holds is that radio is an extremely important tool of communication during emergencies and is a resource worth further researching, especially around the social and public aspect of radio as there is potential to create an effective and prepared response to disasters.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

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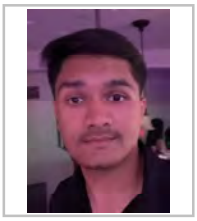
|---|---|---|---|
| **Name:** | Eric Fagan | | |
| **Academic Institution:** | University of Maryland College Park | **Major:** | Civil Engineering |
| **Academic Standing (Sept. 2022):** | Senior undergratuate in Fall 2023 | | |
| **Future Plans (School/Career):** | Attend graduate school and pursue a Master's degree, then try to find employment as a civil engineer | | |
| **NIST Laboratory, Division, and Group:** | Engineering Labs | | |
| **NIST Research Advisor:** | Dr. Dustin Cook | | |
| **Title of Talk:** | Development and Utilization of a Database on Nonstructural Component Damage | | |

**Abstract:**

Nonstructural components are important to keep in mind when trying to recover buildings after seismic events, as their high cost and susceptibility to damage lead to them having a much larger impact on the functionality of the building than initially expected. However, nonstructural components are one of the most overlooked parts of performance-based earthquake engineering. While the performances of some nonstructural components have been studied previously through experiments and post-event analysis, the availability of such data for use in simulations is sparce. In this presentation, I will discuss an ongoing effort to collate studies of experimental, analytical, and historical data on damage to nonstructural components via seismic events into one database to improve accessibility and data reuse for practitioners and researchers. This database can consequently be used for a variety of purposes, ranging from building designs to cross-referencing sources for research, thus allowing for an improved state-of-practice for nonstructural seismic performnce modeling and expediting the evolution of safer and more reusable nostructural components in buildings.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|
| **Name:** Varadraj Chavan | | |
| **Academic Institution:** | Georgia Institute of Technology | **Major:** Biomedical Engineering |
| **Academic Standing (Sept. 2023):** | Sophomore | |
| **Future Plans (School/Career):** | Graduate School | |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Materials and Structural Systems Division, Polymeric Materials Group | |
| **NIST Research Advisor:** | Lipiin Sung | |
| **Title of Talk:** | Breaking Down Plastics: Unveiling the Degradation Process | |


**Abstract:**

The pervasive presence of nanoplastics in the environment poses a growing concern for ecosystem health and human welfare. In this research project, we focus on addressing this issue by investigating the weathering of plastic using the NIST SPHERE (Simulated Photodegeneration via High-Energy Radiant Exposure) weathering device. Our primary objective is to systematically generate model nanoplastic molecules from water bottles, which can be utilized for improved identification and characterization in subsequent testing. To achieve this goal, we employ a comprehensive approach involving both top-down and bottom-up methodologies. Cryo-milling is utilized in both methods to reduce plastic samples to the nanoscale we are looking for. Additionally, the SPHERE device is utilized to simulate the effects of photodegradation, subjecting the plastic samples to approximately 24 days of UV exposure. This duration is chosen to approximate the equivalent of a year of natural sunlight exposure in a typical year in Florida.

Throughout the exposure period, the plastic samples are periodically retrieved for various analyses. Fourier-transform infrared spectroscopy is conducted to study chemical changes, while differential scanning calorimetry is employed to measure physical changes. Color and gloss testing are performed to assess alterations in color appearance. By employing these techniques, we aim to systematically investigate the behavior of plastic under simulated weathering conditions, providing insights into the chemical, physical, and visual changes that occur. Through this research, we seek to enhance our understanding of the behavior and fate of nanoplastics in the environment. The findings from this study will contribute to the development of effective strategies for the identification, monitoring, and mitigation of nanoplastics, ultimately safeguarding environmental ecosystems and human health.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Braedon Mullin

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

**Academic Standing (Sept. 2023):** Sophomore


**Future Plans (School/Career):** Pursue a Master's Degree

**NIST Laboratory, Division, and Group:** Engineering Laboratory, Division 732, Group 2

**NIST Research Advisor:** Natascha Milesi Ferretti

**Title of Talk:** In-Situ Calibration of Differential Pressure Transducers


**Abstract:**

Reducing pressure loss in pipes leads to more efficient energy use. The NIST Pressure - Flow Rate (PvQ) laboratory is designed to test pipe fittings, which can cause significant pressure loss by creating separating and secondary flows. The PvQ lab uses differential pressure transducers to compare the pressure before a pipe fitting to pressures at increasing distances after the fitting. In order to conduct accurate research, transducers used to measure the pressure must be reliably calibrated. The objective of this SURF project was to prepare for future testing of the pressure loss associated with a variety of pipe fittings by designing and installing a calibration system. The calibration system was configured to be permanently integrated into the existing pressure loss test rig in the lab so that the transducers may be calibrated whenever needed. The approach involved placing a tall water column that would generate up to 10 psi of pressure, and connecting it to both the differential pressure transducers from the rig and a factory calibrated pressure transducer. This permits a comparison of the voltage signals that the differential pressure transducers emit to the values of pressure that the factory calibrated transducer returns, due to them receiving the same pressure from the water column. A LabVIEW program was written to automate the system with solenoid valves and simultaneously collect data from all transducers. Then it uses a linear regression analysis to establish the calibration curve for converting voltage returned by the differential pressure transducers to a pressure value.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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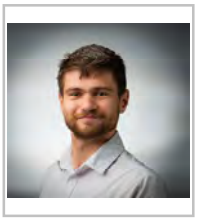
|---|---|
| **Name:** | Bradley Estacio |
| **Academic Institution:** | Illinois Institute of Technology |
| **Major:** | Computer Engineering |
| **Academic Standing (Sept. 2023):** | Graduated Spring 2023 |
| **Future Plans (School/Career):** | Apply to graduate school. |
| **NIST Laboratory, Division, and Group:** | Engineering Lab (EL) |
| **NIST Research Advisor:** | Parastoo Delgoshaei |
| **Title of Talk:** | Efficient and Compliance Check of HVAC information for Two NIST Facilities |

**Abstract:**

With semantic models, advanced analytics techniques, such as data mining, machine learning, and artificial intelligence, can be applied more effectively. In this project, we are focusing on developing and upgrading two semantic models of labs with the engineering lab at NIST to be compliant with the new emerging standard ASHRAE 223P. The two semantic models looked at were the models for Heat Pump Laboratory (HPL) and Intelligent Buildings Agents Laboratory. Up-to-date models can give users insight as to the equipment topology and sensor placements along the pipes, ducts, and spaces in a building. We used the Resources Description Framework (RDF) to develop these models and use SPARQL as a query language to provide insight and answer questions essential to different building applications such as Fault Detection and Diagnostics, commissioning, and smart grid.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Tague Carlyon |
| **Academic Institution:** | Middle Tennessee State University |
| **Major:** | Aerospace Engineering Tech and Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Pursue Masters of Aerospace Engineering |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, 733, Fire Research |
| **NIST Research Advisor:** | Kevin McGrattan |
| **Title of Talk:** | Predicting Wildfire Spread using Computational Fluid Dynamics |

**Abstract:**

For some time the Coast Guard has been able to predict where an individual who needs rescuing may have drifted off into the ocean using a mix of finite element analysis and computational fluid dynamics. Can we offer the same techniques to firefighters battling forest fires? Using Geographic Information System (GIS) mapping and databases created by the U.S. Geological Survey, Weather Service, Forest Service and others, it is possible to gather terrain and weather data to predict the propagation of a wildfire from its point of origin with a fire model like the NIST Fire Dynamics Simulator. A case in point is the Chimney Tops 2 fire that occurred in the vicinity of Gatlinburg, TN, in 2016. Burning in total 4,600 hectares (11,410 acres) of the Great Smoky Mountains National Park, it presents an excellent opportunity to evaluate the predictive capability of the fire model in complex terrain. The terrain presents a unique challenge as it works in conjunction with the fire to create very high wind speeds reported to be upwards of 22 m/s (50 mi/h) which has a major impact on how the fire spreads.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Jaskaran Gill |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Pursue a career in software development |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Fire Research Division, 733 |
| **NIST Research Advisor:** | Randall McDermott |
| **Title of Talk:** | Online Documentation for NIST Fire Dynamics Simulator (FDS) |


**Abstract:**

The Fire Dynamics Simulator (FDS) is a computational fluid dynamics simulation software built at NIST. It is specifically designed to evaluate building fire protection systems and the evolution of fire spread. The documentation for Fire Dynamics Simulator (FDS) is primarily available in PDF format. There are issues concerning the PDF format such as large file sizes, improved accessibility for users, and visual appeal. With the FDS validation guide reaching over a thousand pages a proposed solution is necessary to improve its usability. In order to solve these issues conversion of the PDF documents into online documentation was explored. Many modern software packages utilize online documentation as it offers several advantages over traditional formats like PDFs. An example of such software is Sundials, an open-source software library that provides a suite of solvers for solving systems of ordinary differential equations (ODEs) and differential algebraic equations (DAEs). A key feature included in Sundials online documentation is the cross-platform capability which allows the documents to adapt and respond to different screen sizes and resolutions. To overcome the issues regarding the PDF documentation we utilized Sphinx, an open-source documentation generation tool widely used by software developers. The popularity of Sphinx within the Python programming community and other software projects attests to its effectiveness. By using markup languages such as reStructuredText and markdown Sphinx can generate HTML, CSS, and JavaScript code for functional websites. Additionally, the project evaluates the feasibility of transferring LaTeX math documentation to the new online format. Since the original documentation was written using LaTeX, preserving the mathematical expressions and formulas is crucial for maintaining the integrity of the content. However, certain challenges were encountered when utilizing Sphinx. Difficulties arose specifically with regard to implementing LaTeX math, cross-referencing, and equation indexing within the documentation. In order to facilitate collaboration and version control, a dedicated GitHub repository was created for the online documentation.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Tiller Van Doren |
| **Academic Institution:** | Reed College |
| **Major:** | Physics/Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | 3rd year |
| **Future Plans (School/Career):** | Graduate college |
| **NIST Laboratory, Division, and Group:** | EL, Fire Research Division 733 |
| **NIST Research Advisor:** | Isaac Leventon |
| **Title of Talk:** | Fire Research Problem: Construction of Flame Spread Apparatus |


**Abstract:**

An important piece of information for a first responder to know is how big a fire is and how much it will spread. It is hard to scientifically quantify the size of a fire because of varying fire intensity and constant movement of the flames themselves. As a result, these properties are generally equated to how much heat an object will release through burning, also known as that object's heat of combustion. My main project over the summer is to measure the heat of combustion along with other thermo-physical properties of various materials. The materials I am studying are primarily plastics and foams which are commonly used in construction and manufacturing.

We use a microscale combustion calorimeter (MCC) to measure the thermal-physical properties of a tiny sample which weighs only 5mg by heating it in a controlled environment. After determining the sample's properties, we can simulate how fire will behave as the material burns and compare these simulations to full scale fire tests to create a quantitative model of fire growth that will be used to establish a publicly accessible material flammability database.

I am also spending my summer assisting in the construction of a lab apparatus which will be used for fire spread tests. These tests will be done with panel samples on the scale of a few square feet and less than an inch thick. One edge of the panel will be ignited and a mass balance along with various heat flux gauges are used to observe the fire and material behaviors as the fire spreads across the sample.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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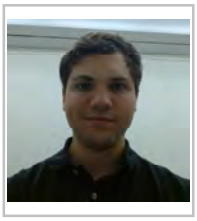
|---|---|
| **Name:** | Nicholas Redford |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Aerospace Engineering |
| **Academic Standing (Sept. 2022):** | Junior |
| **Future Plans (School/Career):** | Finish Undergrad, find engineering job, considering pilot school |
| **NIST Laboratory, Division, and Group:** | Engineering Lab, Fire Research Division, 223 |
| **NIST Research Advisor:** | Isaac Leventon, Michael Heck |
| **Title of Talk:** | Interpolation of Flammability Behaviors through Different Materials |


**Abstract:**

Material Flammability behavior is a field of science that hasn't been studied for much long; only since the fifties have scienctusts researched ignition patterns burning rates throughout different materials. Despite this, learning how these bahaviors work is vital to understand and adapt on current technologies, whether it's testing the igniton growth of a small scale fire to a large one on a family home, or measing the effects of differnents materials that could prevent serious physical and enviornmental damage.

I am focusing on the development and application of the capabilities (experimental & computational analysis tools) to enable quantitative prediction of material flammability behavior (e.g., ignition, steady burning, fire growth). These tests will be run via a wide scale of plastics to common peats samples found in forests prone to burning. I will be measing the energy the material releases when burnt, as well as how much is left after the experiment is finished.

In addition I am building, calibrating, and running tests in some of the bench scale apparatus needed to maintain these capabilities, with a special emphasis on mg- and g-scale thermal decomposition experiments.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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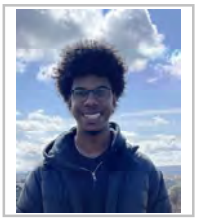
|---|---|
| **Name:** | Yehoshua Halle |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate School |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Systems Integration Division, Digital Twin Lab |
| **NIST Research Advisor:** | Dr. Guodong Shao |
| **Title of Talk:** | Digital Twin Development for an Automated Robot Workcell |

**Abstract:**

Digital twins have become an important research area in manufacturing because of their utility in applications such as status monitoring, analysis, real-time control, predictive maintenance, and optimization. A digital twin is a digital representation of a physical system that accurately models properties of interest of the system in real time. The digital twin should communicate with its physical counterpart bidirectionally, i.e., collect data from and send control commands to the physical system. The goal of the SURF project is to develop a digital twin for a UR5e robot arm performing a pick-and-place operation. Implementation of the digital twin follows guidelines provided by the recently published ISO standard ISO 23247- Digital Twin Framework for Manufacturing. A communication protocol, MTConnect, has been used for real-time equipment data collection. Computer Aided Design (CAD) data of the robot and its gripper are stored in the standard STEP format. The CAD models are imported into MATLAB Simscape, where the arms' physical dynamics are also modeled. Simulink Desktop Real-Time is used to send real-time data to and from the simulation. The completed digital twin can be used for monitoring the state of robot operations and detecting discrepancies between the ideal and actual performance of the physical entity. The project exemplifies the applications of relevant standards for digital twins. Lessons learned from this implementation will provide valuable insight into the digital twin development process and inform development of relevant standards.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

| | |
|---|---|
| **Name:** | Ivon Eric Charlery Jr. |
| **Academic Institution:** | The Catholic Univresity of America |
| **Major:** | Electrical Engineering Computer Science |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Complete my undergraduate degree and gain work experience in the EECS field. |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group |
| **NIST Research Advisor:** | Dr. Guodong Shao |
| **Title of Talk:** | Digital Twin of Desktop Computerized Numerical Control Machine |


**Abstract:**

The digital twin technology has opened many doors by providing a virtual counterpart of physical machines. This virtual counterpart, i.e., digital twin, can collect and analyze real time data of a physical machine. The use of digital twins provides manufactures various capabilities such as predictive maintenance, enhanced monitoring, and quality control.

In this project a digital twin of a desktop computerized numerical control (CNC) machine tool, Pocket NC v2-10, is developed, based on ISO 23247, Digital Twin Framework for Manufacturing. Another standard, MTConnect, is used to collect the real time operational data of the machine tool. This enables the synchronization between the physical machine and its digital twin. A few test cases have been created to validate the developed model of the machine so users may observe the status and operation of the machine.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | William Stiller |
| **Academic Institution:** | Penn State Erie, The Behrend College |
| **Major:** | Digital Media, Arts, and Technology |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate School in Information Technology or related field |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group |
| **NIST Research Advisor:** | Guodong Shao |
| **Title of Talk:** | Hierarchical Data Structure Development to Support Digital Thread and Digital Twin Applications |

**Abstract:**

Digital twins are an effective method for digitally representing, analyzing, and optimizing a physical manufacturing element. However, it may be a challenge to collect, process, and model all the required data in different formats from various sources. For example, to develop a digital twin of a part being manufactured, data required may include the data from multiple stages of the product lifecycle, from design, to engineering, manufacturing, inspection, and use. Within each stage, specific data standards and formats may be used, and it has proven challenging to relate the different information gathered to a single part.

A digital thread is a communication framework that would assist in linking the data to support the development of a digital twin. Currently, no framework exists that can easily and efficiently support the storing, representation, and exchange of such data in the digital twin Lab. This project focuses on creating such a framework by working with novel data storage solutions to represent product lifecycle data while leveraging digital twin applications in manufacturing. A use case of the selected structure is developed to represent data from product lifecycle stages and demonstrate digital twin applications using the data structure.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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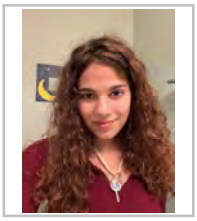
|---|---|
| **Name:** | Vladimir Ignacio Alvarado |
| **Academic Institution:** | Montgomery College |
| **Major:** | Civil Engineering |
| **Academic Standing (Sept. 2023):** | Undergraduate Student |
| **Future Plans (School/Career):** | Associate of Science Degree and then pursue a undergraduate degree at acredited four-year institute. |
| **NIST Laboratory, Division, and Group:** | Engnineering Laboratory, Systems Integration Division 734 |
| **NIST Research Advisor:** | Peter O Denno |
| **Title of Talk:** | Using Large Language Models to Help Formulate Scheduling Problems |

**Abstract:**

Manufacturing scheduling problems can be costly. Since scheduling problems can often be modeled as combinatorial problems, we can use domain-specific languages (DSLs) like MiniZinc, which optimizes combinatorial problems to find solutions. Because MiniZinc is an esoteric language, there is a divide between the engineer, who is acting as an expert in their field, and their understanding of MiniZinc. By using a large language model (LLM), we seek to bridge this divide: developing a classification of the sentences in an engineer's description is one step in achieving this. The joint work of the engineer and the LLMs allows the engineer to " be kept in the loop" during the formulation of the MiniZinc model. In this SURF experience, we seek effective classifications. We do this by investigating how our classifications and the LLMs classification of the user's prompts can serve our purpose of bridging the divide.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Tali Schlenoff |
| **Academic Institution:** | University of Maryland - College Park |
| **Major:** | Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Attend graduate school for mechanical engineering, and ideally work in engineering design |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Division/Group 735.13 |
| **NIST Research Advisor:** | Jeremy Marvel |
| **Title of Talk:** | InterFace the Facts |

**Abstract:**

Robots are designed to aid humans with a variety of tasks, especially those that need a lot of precision/repetition or could put people in harm s way. These are some of the many reasons why there has been such a large push to integrate robots into industry. However, robots are very complex, and it cannot be assumed that every industry worker that will be operating them has an engineering degree and complete understanding of how each robot works. The way to get around this is to create an appropriate user interface (UI) that can accommodate whoever may be using it. My work in the project centered around doing research to figure out criteria for such an interface. My attention was mainly toward mobile devices since they are analogous to those interfaces that are most likely to be used for the average industry worker controlling robots. From here, I considered and looked into the physiological and psychological necessities/preferences for those with and without physical or mental disabilities. I also accounted for the cultural differences for, what we consider, the five major manufacturers (America, Japan, Germany, Britain, and Australia/New Zealand). This research will enable the production of a user interface that can assist as many industry workers as possible, regardless of their background or ability.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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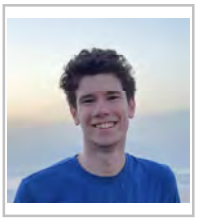
|---|---|
| **Name:** | Parker Liposky |
| **Academic Institution:** | Embry-Riddle Aeronautical University |
| **Major:** | Unmanned Aircraft Systems Science |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Finish undergraduate degree at ERAU |
| **NIST Laboratory, Division, and Group:** | Engineering Labratory, Intelligent Systems Division, Sensing & Perception Systems Group |
| **NIST Research Advisor:** | Dr. Kamel Saidi |
| **Title of Talk:** | Aerial Drop Tests Research |


**Abstract:**

The National Institute of Standards and Technology (NIST) has been developing testing standards for emergency response robots and drones under the Intelligent Systems Division (ISD). The ISD at NIST works closely with other government organizations including the Federal Aviation Administration (FAA) to develop standard test methods and promote governmental research between the two agencies. The FAA is responsible for providing the safest and most efficient aerospace in the world, and accomplishes this mission by adopting the rules and legislation which govern national airspace (NAS) in the continental United States.

NIST has been collaborating with the FAA by conducting tests related to vital research topics. This summer, I will be working with my student mentor, Dr. Kamel Saidi, and his team of international research scientists to develop testing protocols for dropping drones from aerial vehicles. Testing environments will include an indoor and outdoor testing facility. The indoor testing facility will present us with unique data outcomes due to the lack of external factors such as wind. Indoor test apparatuses will be much more controlled in measuring drop speed and kinetic energy. The outdoor testing facility will be representative of a true standard operating environment due to natural environmental factors such as wind, and is where the majority of our tests will be conducted.

The main purpose of our research will be to evaluate and quantify the impact of drones being dropped from different altitudes. In the United States, drones present an increasing threat to the general population. With the knowledge of how commercially available drones perform under different conditions and altitudes, the FAA will be aware of the various dangers they present and therefore be able to adjust legislation accordingly. For the purpose of this project, our research at NIST will directly



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Ethan Sundel |
| **Academic Institution:** | University of Pennsylvania |
| **Major:** | Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Finish my bachelor's degree and pursue a master's degree |
| **NIST Laboratory, Division, and Group:** | Engineering Laborotory, Intelligent Systems Division, Emergency Response Robots and Drones |
| **NIST Research Advisor:** | Adam Jacoff |
| **Title of Talk:** | Standardized Testing and Validation of Emergency Response Systems |


**Abstract:**

Emergency responders, military organizations, and others often risk their lives in order to protect the public. While doing this their only defense is personal protective equipment. Emergency response robots and drones provide a partial solution to this problem, allowing unmanned vehicles to intervene in certain situations where it might prove dangerous or even fatal to a human. NIST is developing a comprehensive set of standardized test methods to evaluate the performance and pilot proficiency of these systems, enabling pilots to effectively operate unmanned aerial and ground vehicles during emergency situations. NIST's testing procedures involve the use of cost-effective and easily fabricated apparatuses made from wood and plastic buckets. These apparatuses are carefully designed to assess pilot and system proficiency across various crucial aspects including acuity and maneuverability. These tests have the potential to incur life-saving impacts and significantly improve response efficiency.

In the initial phase of this project, I observed how NIST is transitioning from 8-inch diameter buckets to 4-inch. This change allows for the simplification of the fabrication process, more effective storing of apparatuses, and cheaper cost to create. To validate this change, I conducted some of NIST's existing aerial tests on both the old and new setups, took data and analyzed it. The goal was to ensure that these new tests continue to meet the rigorous standards set by ASTM international and can be adopted as universally recognized and standardized test methods.

The second part of my project involved integrating a range of cameras, sensors, and tools onto a ground Explosive Ordnance Disposal (EOD) robot. This robot, the Telerob Telemax Evo Pro, serves as a validation platform for our ground tests. I attached and tested eight of these devices to explore the robot's complete capabilities. The insights gathered from this experimentation will contribute to the development of more comprehensive and detailed standardized test methods. Ultimately, the advancements achieved through these standardized test methods will benefit emergency responders worldwide.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Brian Maloney | |
| **Academic Institution:** James Madison University | **Major:** Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | I plan to pursue a career in engineering and go to graduate school. |
| **NIST Laboratory, Division, and Group:** | Engineering Lab, Intelligent Systems Division, Agility Performance of Robotic Systems |
| **NIST Research Advisor:** | Anthony Downs |
| **Title of Talk:** | ROS Integration with Agile Performance Robotic Systems |


**Abstract:**

There is an increasing interest in the utilization of the Robot Operating System (ROS) and its successor, ROS2, within the context of robotics applications in U.S. manufacturing. ROS, an open-source software framework, offers a comprehensive suite of tools and libraries that enable advanced robot programming. This SURF project aims to explore and leverage the potential of ROS2 to enhance robotics operations in a manufacturing setting. The primary objective of this project involves converting the lab into an environment that runs Java-based demonstrations for both simulated and in-person robots. This entails gaining proficiency in programming robotic systems using ROS and ROS2, understanding their underlying principles, and effectively implementing them within a laboratory environment. Additionally, this project focuses on improving the capabilities of the robotics setup by integrating a conveyor belt through the use of a Programmable Logic Controller (PLC) and the TwinCAT software to enable seamless interaction with an external ROS node. This integration will enhance the flexibility, coordination, and efficiency of robotic operations on the manufacturing floor.

Throughout this project, a series of experiments will be conducted to evaluate the integration of the conveyor belt with the PLC and its compatibility with ROS. The project will involve further development of existing communication protocols, establishing reliable data exchange between the ROS ecosystem and the PLC, and ensuring proper synchronization and coordination of robot movements with the conveyor belt's speed and position. The outcomes of this project will contribute to the growing body of knowledge on ROS and ROS2 integration within the manufacturing sector and at NIST. The successful implementation of the proposed enhancements and integration will provide valuable insights and practical solutions for future deployments of ROS-based robotic systems in US manufacturing, leading to improved automation and efficiency in industry.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Khoa Nguyen |
| **Academic Institution:** | University of Maryland: College Park |
| **Major:** | Mechanical Engineer |
| **Academic Standing (Sept. 2023):** | Undergraduate Sophomore |
| **Future Plans (School/Career):** | I planned to attend graduate school after finishing my 4 years |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Division: 753.13, Group: |
| **NIST Research Advisor:** | Shelly Bagchi |
| **Title of Talk:** | Collection, Analyzation, and Vizualizing of RGB and Depth Data for Human Study |


**Abstract:**

Later in the year, the Performance of Human-Robot Interaction Project (PHRI) will conduct a human study to test different interfaces' usability, functionality, and comprehensibility in assisting participants in teleoperating a collaborative industrial robot. The study will attempt to evaluate which interface results in better task performance for a manufacturing task, as well as better user experience. With multiple participants, there comes the need to reliably automate the process of data collection, analysis, and visualization. A script is being developed to collect and process datasets taken from user inputs on three types of interfaces. These include the built-in robot teach pendant, an augmented reality headset, and a virtual reality teleoperation tool.

The User Interface (UI) of the data collection script will stream and record RGB video and color-coded depth maps using the Intel RealSense Depth Camera D435i. After each recording, a ".bag" file is extracted which contains depth images, RGB images, and infrared frames in raw format. These are converted into point cloud format which are mapped onto 3D space to yield a rough representation of the topography. In improving the quality and accuracy of the 3D model, recordings from multiple cameras will be captured and potentially synced together to accurately capture the topography as well as minimizing blind spots. Optimization and implementation of this script can, for instance, aid researchers in visualizing the position an object occupies in 3D space over time. For this study, it facilitates the quantitative analysis of how different study participants accomplished the task.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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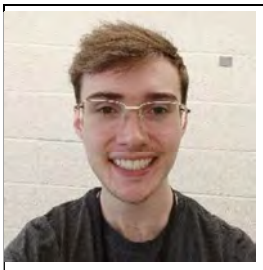
|---|---|
| **Name:** Noam Peled | |
| **Academic Institution:** University of Maryland | **Major:** Computer Engineering |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Masters in Computer Engineering or work in R&D department of forward thinking company |
| **NIST Laboratory, Division, and Group:** | Engineering Lab 735.12 |
| **NIST Research Advisor:** | Helen Qiao |
| **Title of Talk:** | Real-time Pose Measurement to Support Robot Inspection |

**Abstract:**

The use of robots in high-precision applications has been increasing, for example, robot real-time inspection. The capture, analysis, and real-time feedback of inspection results in users making the best decision on time. For robot inspection, the robot is performed as a carrier of the inspection sensor. The robot's accuracy needs to be assessed and the dynamic motions need to be measured to satisfy the requirement of registering inspection data. The robot arm's position and orientation information are used to register the sensor data for full 3-D analysis. NIST has developed a smart target to support the precise measurement of a robot's position and orientation. The target is mounted on the object (e.g., end effector or tool of a robot arm) whose accuracy is to be ensured in order to measure and track the object's six-dimensional position and orientation. To capture images for calculation, two pinhole cameras are used and a relative rotation and translation matrix between the cameras is produced. This enables triangulation for accurate position calculations. The first item to finalize is calibration testing and documentation. The second item is debugging and iteration of the real-time position calculation algorithm.



# SURF Student Colloquium

NIST – Gaithersburg, MD August 1-3, 2023

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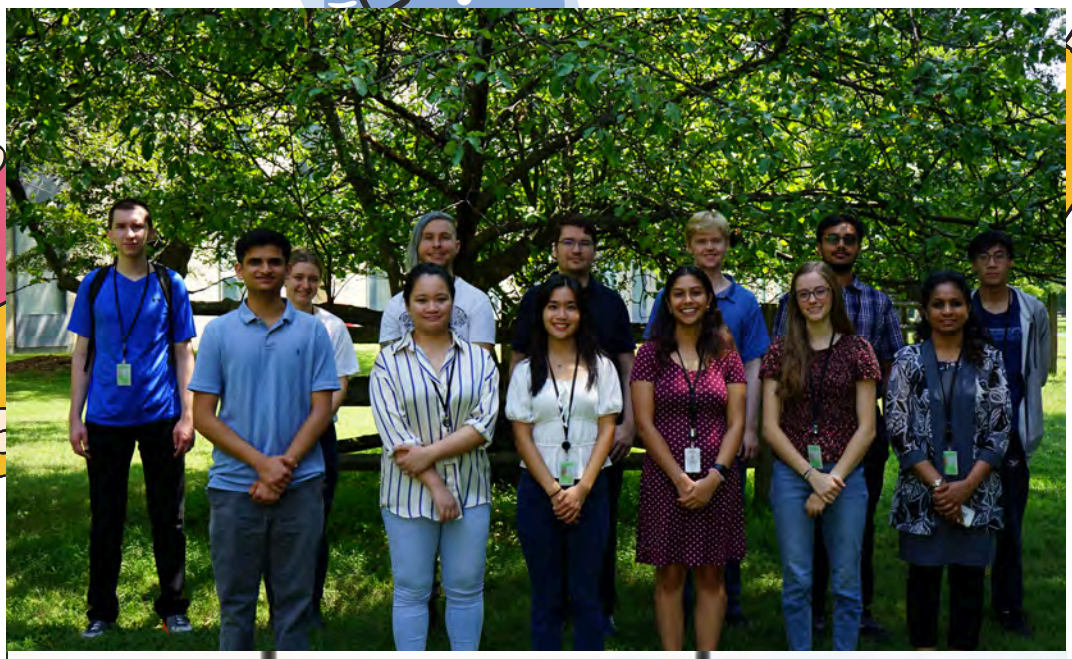
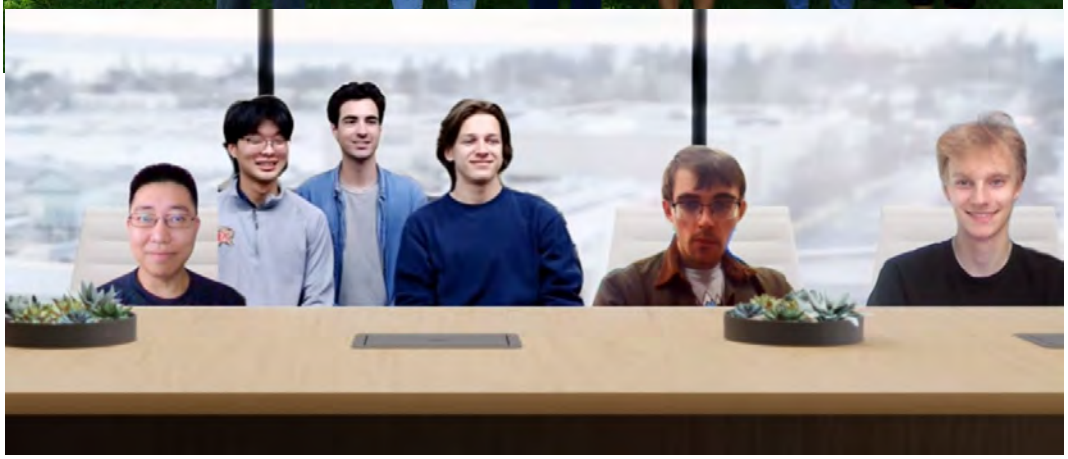
|---|---|
| **Name:** Elijah Martin | |
| **Academic Institution:** University of Maryland | **Major:** Electrical Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate from the University of Maryland, and potentially go to graduate school. |
| **NIST Laboratory, Division, and Group:** | Engineering Laboratory, Intelligent Systems Division (735), Production Systems Group (15) |
| **NIST Research Advisor:** | Felix Kim |
| **Title of Talk:** | Developing a Custom Spin Coater Using a Microcontroller and 3D printing |


**Abstract:**

The purpose of this project is to design and construct an inexpensive and custom spin coater using off-the-shelf components. Commercial spin coaters can be costly to purchase and are usually optimized for standard wafers, and making a custom design allows us to make a spin coater that can use custom samples at a fraction of the cost. Spin coaters are used to deposit thin films of material on flat substrates by spinning solutions such as photoresists, nanomaterials, and gels- at high speeds, and centrifugal force from the spinning causes a uniform film with thickness inversely proportional to the speed. Spin coaters are applied in various fields including semiconductors, nanotechnology, material science, and microfluidics. In our case thin films of photoresist on custom substrates can have a pattern be transferred upon them through a maskless lithography process, and then etched to fabricate controlled defects for X-ray computed tomography (XCT) defect detection studies. To create the spin coater, common parts for DIY hobby electronics were used such as a brushless direct current (BLDC) motor, a microcontroller, and a touchscreen display. The design is based primarily off the MAASI spin coater design (doi.org/10.1016/j.ohx.2022.e00316): this existing design was modified to improve its functionality, to use components available from US retailers, and to accommodate larger and different sized samples. The sample holder can easily be built and replaced for different substrates. The process of building the spin coater is an iterative process involving computer aided design (CAD), polymer 3D printing, post processing 3D prints by cutting and sanding, soldering electronics and verifying their function, and coding using the Arduino IDE. The design and manufacturing process, BLDC motor control using a microcontroller and electronic speed controller, and test measurements made on thin films of PDMS, or photoresist will be discussed. The knowledge learned in the project can be easily applied to different applications such as unmanned aerial vehicles or robotics.





# Information Technology Laboratory 2023

**Summer Undergraduate Research Fellowship (SURF) - 2023 Participants**

*(in the order of the Colloquium schedule)*

Information Technology Laboratory (ITL))

*Katherine Harvey:* Reaction Limited Approximations of Biosensor Field Effect Transistor Experiments

*Vivian Xiao:* BioFET Sensitivity Analysis

*Luke Hawranick:* Inter-node Communication Performance Tuningg

*Dongxing He:* Fiber-link characterization of quantum network fibers using single photon detection

*Michael Szilagyi:* Converting OpenGL Shaders to Run in ParaView Visualization Software

*Morgan Ko:* Making 3D Formats Accessible for Scientific Data Using glTF

*Leon Jia:* Characterization of Quantum memories and SiC-based Quantum Devices

*Mikhail Krepets:* Modifying the Walk on Spheres algorithm to see if it would make ZENO faster

*Faadil Shaikh:* Implementation of Fastest Closest Point in the West to accelerate Capacitance calculations using ZENO

*Thomas Wolcott:* Designing an interface for the B Spline R-matrix codes

*Peter Burbery (virtual):* Translating Mathematica expressions in q-calculus to LaTeX

*Noah Schulman:* Evaluating Generative AI Audio Deepfake Tools

*Kaylin Yeoh:* An Evaluation of Synthetic Data Generation Methods for Tabular Data

*Luke Zic:* Video Retrieval Evaluation Leaderboard Development

*Marilyn Nguyen:* : Implementations of Mobile Driver's Licenses and Everyday Documents

*Alex Dai:* Exploring Suitable Structures to Store mDoc Field Data

*Brian Chen (virtual):* Graph Database for NIST Cybersecurity Publication Citation Relationship

*Jayden Crosby (virtual)*: Chatbots and Search

*Francsi Durso (virtual):* A Combinatorial Approach to Explainable AI

*Navya Gautam (virtual):* Creating an Enriched Cybersecurity Risk Dataset with Visualizations to Analyze and Evaluate Cyber Risk Incidents

*Anthony Malysz (virtual):* Next Generation Policy-as-Code

*John Guerreio (virtual):* Understanding Memory Related CWE Entries with Bugs Framework

*Zach Benton (virtual):* CNN-based texture directionality detection

*Vidhata Jayaraman (virtual):* Surprising Sentences

*Ishaan Bhardva:* Impact of Weather Parameters on Path and Clock Delay in Quantum Networks

*Kathryn Butziger:* Comparison of AI Model Attribution Methods

*Carina Carino:* Deep Learning-Based Viral Plaque Detection in Label-Free Phase Contrast Images

*Ryan Trask:* Correction of the Meniscus Effect in Biological Samples with Convolution Neural Network Models

*Stanley "Troy" Conklin:* Creating Abstractions for Real-time Image Processing

*Sonika Sharma:* Confirm That 25 747 New Programs Can Replace the 32 003 Programs of the Old C# Test Suite

*Saahil Singh:* Mapping Categorical Emotions and Dimensional Attributes from Text Data to Sentiment Scores

*Max Filliben:* Web-based Statistical Tools for Radionuclidic SRMs

*David Sadek:* Errors in Variables Regression Models

*Femina Amoo:* Evolution of cybersecurity education and workforce development

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023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|---|---|
| **Name:** | Katherine Harvey |
| **Academic Institution:** | Hillsdale College |
| **Major:** | Applied Mathematics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | TBD |
| **NIST Laboratory, Division, and Group:** | ITL, Applied and Computational Mathematics Division, Mathematical Analysis and Modeling Group |
| **NIST Research Advisor:** | Ryan Evans |


**Title of Talk:** Reaction Limited Approximations of Biosensor Field Effect Transistor Experiments


**Abstract:**

A Biosensor Field Effect Transistor (BioFET) is a modern medical testing device that shows great promise to providing access to quick, reliable, less expensive medical testing. These devices consist of a small biochemical sensor in a chamber that measures the concentration of a chemical on its surface. Under physically relevant experimental conditions, BioFET's behavior can be well described and predicted with an integrodifferential equation (IDE) as a function of this sensor concentration, B. Numerically, results can be averaged to compare to experimental data; however, due to the complexity of the model, this is computationally expensive. This motivated the decision to employ several approximation methods to reduce the problem's complexity. We derived a perturbation expansion for B and an effective rate constant (ERC) equation, accurate to the order of the Damköhler number squared, for small Damköhler numbers. The ERC equation proves useful because it reduces the IDE to an ordinary differential equation (ODE) in terms of the spatial average over the sensor. Further, the parameter values that describe the properties of the chemical reactant used in the experiment can be optimized to minimize the error between the experimental data and the model. These optimized parameters can then identify the chemical that was used. The Damköhler number describes the ratio between the rate of reaction and the rate of diffusion; hence, small Damköhler number approximations are relevant to experiments where the rate of diffusion is significantly larger than the rate of the reaction. It was shown that the difference between these two approximations is on the order of the Damköhler number squared.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Vivian Xiao | |
| **Academic Institution:** University of Pennsylvania | **Major:** Computer Science |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | School: Pursue a higher degree in Computer Science/Math<br>Career Interests: AI/ML, Data Analysis, Statistics, Software Engineering |
| **NIST Laboratory, Division, and Group:** | Information Technology Lab (Applied and Computational Mathematics Division) |
| **NIST Research Advisor:** | Dr. Anthony Kearsley |
| **Title of Talk:** | BioFET Sensitivity Analysis |

**Abstract:**

Biological Field Effect Transistors (BioFETs) have gained significant attention for their potential in medical applications, including biomarker detection and drug monitoring. Accurate modeling of BioFET performance is crucial for optimizing their design and understanding their behavior under different conditions. This project focuses on the sensitivity analysis of two BioFET models: the faucet model and the droplet model. The name of the model reflects the manner in which target molecules are introduced into the sensor. The faucet model represents continuous injection across the entire width of the sensor, while the droplet model simulates injection at a single point. To quantify the impact of various parameters on BioFET performance, a combination of numerical and analytical methods is employed. Techniques such as the finite difference method, partial derivative calculations, and perturbation methods are applied to assess the sensitivities of each parameter. These methods enable the examination of how changes in kinetic rate constants, diffusion coefficients, and the aspect ratios of the biosensor influence the average concentration detected by the biosensor's receptors over time. The findings from this sensitivity analysis will provide valuable insights into the key parameters affecting BioFET performance. By quantifying the sensitivities, it becomes possible to identify critical factors that significantly impact the biosensor's response. This knowledge can guide the optimization of BioFET design and facilitate a deeper understanding of the underlying biological and physical processes involved.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Luke Hawranick |
| **Academic Institution:** | West Virginia University |
| **Major:** | Mathematics, Computer Science |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Ph.D. program in Algorithms, Combinatorics, and Optimization |
| **NIST Laboratory, Division, and Group:** | ITL, Applied and Computational Mathematics Division, High Performance Computing and Visualization Group |
| **NIST Research Advisor:** | Dr. William George |
| **Title of Talk:** | Inter-node Communication Performance Tuning |

**Abstract:**

Efficient inter-process communication is crucial for enhancing the performance of highly parallel large-scale simulations. However, previous research has not thoroughly explored the performance implications between two commonly used schemes in MPI (Message Passing Interface): manual contiguous packing of send buffers and custom MPI datatypes. We have created an environment in C with a message passing routine similar to that of our parallel dense suspension simulator, written in FORTRAN, and have conducted a comprehensive timing analysis utilizing Raritan's High-Performance Computing Cluster, varying the message passing scheme, MPI implementation, the number of processors used, message size, and whether other tasks are performed concurrently with the message passing. The resulting data will be used to analyze efficiency of data transfer through both a comparison of manual packing against the custom type approach and a comparison of message passing times with and without a concurrent task. These findings will allow for greater timing optimization for highly parallel programs which are computation and communication intensive.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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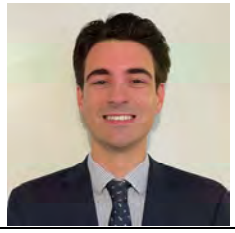
|---|---|---|
| **Name:** Jaden He | | |
| **Academic Institution:** | University of Maryland College Park | **Major:** Physics and Mathematics |
| **Academic Standing (Sept. 2023):** | Sophomore | |
| **Future Plans (School/Career):** | Graduate school in physics | |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory (ITL) | |
| **NIST Research Advisor:** | Thomas Gerrits | |
| **Title of Talk:** | Fiber-link characterization of quantum network fibers using single photon detection. | |


**Abstract:**

Optical Time Domain Reflectometry (OTDR) is a common technique to non-destructively characterize optical fibers and obtain information such as length, attenuation, and location of splices and faults. The technique involves sending laser pulses down an optical fiber and measuring the Rayleigh backscatter with a photo diode, obtaining a trace of light intensity vs. measurement time. Single photon OTDR (v-OTDR) uses single photon detectors that register photon counts rather than light intensity, which allows for better two-point resolution and a shorter integration time to achieve a similar OTDR trace.

In v-OTDR, photon counts are registered in a specified bin size, creating a histogram of photon counts vs. measurement time, which is then converted into decibel loss vs. length along the fiber. If the optical fiber achieves a certain length, the v-OTDR trace will end in a noise floor, where the Rayleigh backscatter is too weak to be registered on a single photon detector.

The purpose of this project is to measure fiber end reflection time, and therefore fiber length, as accurately as possible. We use a superconducting nanowire single photon detector (SNSPD) with near unity detection efficiency and almost no after pulsing or dark count error, a picosecond pulsed laser for precise selection of pulse width and frequency, a modulator to achieve a high extinction ratio, and a calculation of Allan deviation to find the optimal integration time for the lowest end-reflection time measurement error. We found error of ~1mm (3.5ps) in 42km long fiber, confirmed through our Allan deviation calculation, and we will use this technique to measure length fluctuations over time of a deployed fiber from NIST to UMD.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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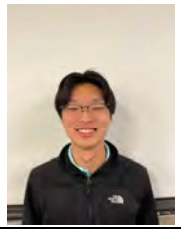
|---|---|
| **Name:** | Michael Szilagyi |
| **Academic Institution:** | George Mason University |
| **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Complete my bachelor's degree in Computer Science and work full-time as a Software Developer |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Applied and Computational Mathematics Division, High Performance Computing & Visualization Group |
| **NIST Research Advisor:** | Judith Terrill and Tere Griffin |
| **Title of Talk:** | Converting OpenGL Shaders to Run in ParaView Visualization Software |

**Abstract:**

A Shader is a user-defined program that runs on a computer's graphical processor (GPU). Shaders are an extremely important part of scientific visualization as they can allow for a variety of complex visual effects, such as intricate 3D models, to be displayed in a resource-efficient manner. The OpenGL Shader Language, glsl, is a widely used high-level programming language used to implement these shaders. These shaders were initially developed to be used within NIST's own High End Visualization (HEV) software, but as we shift to using ParaView, an open-source scientific visualization software, these shaders must be converted in order to be operable. Converting these shaders to work with ParaView involves utilizing VTK, which is the backend of ParaView, to replace the necessary portions of the software's default shaders. A Python-based custom widget allows individual glsl shaders to be loaded within ParaView and automatically converted to the necessary VTK format. This will make using OpenGL shaders in ParaView a seamless task that will greatly improve the efficiency and performance of scientific visualization in our immersive visualization environment (the CAVE).



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|---|
| **Name:** Morgan Ko | | | |
| **Academic Institution:** | University of Maryland | **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Junior | | |
| **Future Plans (School/Career):** | Graduate from UMD with a bachelor's degree in Computer Science alongside a minor in mathematics and persue a career in software engineering or robotics. | | |
| **NIST Laboratory, Division, and Group:** | Information Technology Labratory, Applied and Computational Mathematics Division, High Performance Computing and Visualization Group | | |
| **NIST Research Advisor:** | Judith Terrill, Terence Griffin | | |
| **Title of Talk:** | Making 3D Formats Accessible for Scientific Data Using glTF | | |


**Abstract:**

NIST has been using its own SAVG file format to hold 3D model data for years. There are thousands of files stored using the SAVG format. However, a newer 3D model format has been released called glTF 2.0. This is short for Graphics Language Transmission Format, and was designed by Khronos to be quick to load. In addition it includes a scenegraph and supports a wide range of features including animation, materials, and textures. It is extensible and is widely supported. NIST's High Performance Computing and Visualization Group has many visualization softwares and simulations that use many 3D assets and models. Since glTF files are faster than the older SAVG format, NIST wishes to begin utilizing glTF 2.0 as a new standard for 3D files. In this project, we explore the nuances of the glTF format, create example 3D assets using the glTF format, and create efficient programs using Python to work with glTF assets.

At its core, a glTF asset is a JSON file. For any given glTF asset, it has binary data and a list of attributes that details how the binary data should be interpreted and rendered into a 3D space. All attributes relate to some intricacy of the 3D model or help organize the data. While the attributes are human-readable, the binary data is far from it. During the project we utilized various number conversions in order to match the specifics of the binary format. As previously mentioned, Python was also utilized alongside the pygltflib library in order to easily create and save glTF files through scripting. A larger part of the project has been utilizing this Python library and parsing polygonal SAVG files in order to efficiently and conveniently create a matching polygonal glTF files with ease. This script does this by taking data from each SAVG file and encoding it into a binary file for a glTF asset to read from. This program will be useful in order to utilize the glTF 2.0 format in the future.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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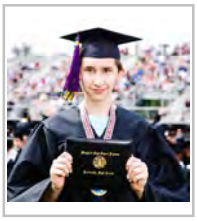
|---|---|---|---|
| **Name:** | Leon Jia | | |
| **Academic Institution:** | University of California, Berkeley | **Major:** | EECS |
| **Academic Standing (Sept. 2023):** | Sophomore | | |
| **Future Plans (School/Career):** | Industry / Graduate School | | |
| **NIST Laboratory, Division, and Group:** | ITL, ACMD, Computing and Communications Theory Group | | |
| **NIST Research Advisor:** | Dr. Lijun Ma | | |
| **Title of Talk:** | Characterization of Quantum memories and SiC-based Quantum Devices | | |


**Abstract:**

Quantum emitters are a crucial component of quantum communication. It is valuable for quantum emitters to emit in the telecom band for effectiveness in modern fiber networks. Vanadium doped silicon carbide is a promising solid state quantum emitter with stable emission in the O band for the 4H and 6H polytypes of SiC, and in the S band for the 3C polytype, which we are particularly interested in. Effective quantum emitters observe photon antibunching, which is important in quantum communication and quantum key distribution. While vanadium ions fully transmit in the telecom band, different silicon carbide polytypes affect the properties of the emissions due to the different substitutional silicon sites. In this study, we plan to investigate quantum properties of vanadium (V4+) doped in 3C, 4H, and 6H polytypes of SiC. We use a piezoelectric controller and single photon detector to iteratively locate each vanadium ion within the SiC lattice. We then characterize the quantum emissions released. Experimental control is conducted in Labview and data analysis conducted in MATLAB. My contributions to the project primarily lie in system control and data acquisition scripts, creation of a GUI for data acquisition, and operation of experimental components. This study will contribute to a wider body of research towards applications in quantum telecom devices and networks.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Mikhail Krepets |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | After completing a BS in CS, I plan to go to grad school and then go into research and/or education. |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Division 771, Mathematical Analysis and Modeling Group |
| **NIST Research Advisor:** | Professor Michael Mascagni |
| **Title of Talk:** | Modifying the Walk on Spheres algorithm to see if it would make ZENO faster. |


**Abstract:**

Walk on Spheres (WoS) is a Monte Carlo algorithm which simulates Brownian motion through the use of spheres. ZENO is a program which uses the WoS algorithm to calculate various traits (such as capacitance and volume) of shapes, usually molecules.

The research task we were assigned this summer was to implement a modification to the WoS algorithm implemented in ZENO and then test whether the speed of ZENO improves or not. The modification is one that slightly over-expands the spheres in the WoS algorithm in hopes of taking less steps while sacrificing a tiny bit of accuracy.

If this modification ends up increasing the speed of ZENO without sacrificing too much accuracy, then it could be implemented in ZENO.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


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|---|---|
| **Name:** | Faadil Abdullah Shaikh |
| **Academic Institution:** | University of Maryland-College Park |
| **Major:** | Computer Science/Mathematics |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Masters in Computer Science |
| **NIST Laboratory, Division, and Group:** | ITL 771 |
| **NIST Research Advisor:** | Micheal Mascagni |


**Title of Talk:** Implementation of Fastest Closest Point in the West to accelerate Capacitance calculations using ZENO


**Abstract:**

In this paper we examine the integration of Fastest Closest Point in the West (FCPW), a C++ Library developed at Carnegie Melon University to perform geometric queries, into ZENO, a software tool developed by NIST researchers to calculate different Chemical properties of given molecular structures. In order to perform calculations, particularly for Capacitance Calculations, ZENO utilizes a Monte Carlo Method known as Walk on Spheres, which requires multiple closest point queries in each individual walk, which is subsequently repeated on the order of 1 million times. This causes some slowdown in the runtime of this program, and as such we can use a faster algorithm to shorten this time manyfold. FCPW is currently the fastest algorithm for such queries, the only problem being the difference in the geometric implementation of the two software.

ZENO's primary base shape is a sphere and structures built as a collection of them, while FCPW s primary base shapes are triangles and triangle meshes of 3D objects. Due to the calculation cost of having to convert spheres into triangle meshes, we decided to directly implement spheres into FCPW in order to integrate ZENO and FCPW together.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Tom Wolcott

**Academic Institution:** University of Maryland, College Park | **Major:** Computer Science & Physics


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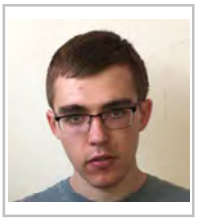
| **Academic Standing (Sept. 2023):** | Sophmore |
| **Future Plans (School/Career):** | I plan continue on to graduate school |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Applied and Computational Mathematics Division, Group 771 |
| **NIST Research Advisor:** | Barry Schneider |
| **Title of Talk:** | Designing an interface for the B-Spline R-matrix codes |


**Abstract:**

The Atomic, Molecular, and Optical Science (AMOS) gateway serves as an online portal, providing researchers and students access to scientific software tools in a browser, where, previously, they would've had to download, compile, and troubleshoot these codes themselves. However, these interfaces are not accessible to new users as they still require in-depth knowledge of the codes. For this reason, the project aims to build powerful, user-friendly interfaces to the codes on the AMOS gateway, starting with the B-Spline R-matrix (BSR) codes. In this vain, an interface to the tRecX program already exists, whose code and design docs greatly informed the overall structure and design used in the BSR interface. These two applications are differentiated, however, by BSR's many inputs and codes, whereas tRecX has a single input and code. The other codes also differ from the tRecX greatly and require their own tailored designs. Specifically, in the case of BSR, its interface requires the ability to upload and view many files while still satisfying the overarching goal of being useful to both new and experienced users.

The interface uses the Django web framework to handle most of the backend, which includes communication with AMOS gateway API, defining and storing data relevant to the interface, and creating its own API to access this data from. The frontend is then handled by Vue, which is able to provide an intuitive interface that then connects to the backend through its API.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Peter Cullen Burbery

**Academic Institution:** Marshall University | **Major:** Computer Science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| **Academic Standing (Sept. 2023):** | Good Standing Dean's List Senior |
| **Future Plans (School/Career):** | Accelerated Masters Degree at Marshall University, then a PhD in Computer Science |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory (ITL) |
| **NIST Research Advisor:** | Howard Cohl, Ph.D |
| **Title of Talk:** | Translating Mathematica expressions in q-calculus to LaTeX |


**Abstract:**

In this talk, we describe efforts using the Wolfram Language to translate computable expressions in Mathematica into LaTeX for q-calculus. For instance, we translate basic hypergeometric series (represented with the Wolfram Language-defined function QHypergeometricPFQ) and various other functions associated with these functions into LaTeX. The expressions that we translate include various combinations of sums (Sum), integrals (Integrate), finite (QPh) and infinite (QPhI) q-shifted factorials, very-well-poised hypergeometric functions (user-defined Wolfram Language functions) and fractions. One challenging task that we have tried to implement in order to provide satisfactory translations, is to rearrange multiplicative sub-expressions which involve the parameter q such that the q is in front. This reflects the importance of the variable q in q-calculus. An example would be to transform p*q*r into q*p*r. The challenge is that Mathematica automatically reorders the output q*p*r to p*q*r and this undoes the transformation. For our test example, the output would be q*pr (* represents noncommutative multiplication with the function NonCommutativeMultiply, which does not reorder to p*q*r). We use List@@ to convert multiplicative sub-expressions like p*q*r into lists such as {p,q,r}, and then use PositionQInFrontOfList to return {q,p,r}. We then transform back to q*p*r with Apply. We use Inactivate. We give functions the attribute HoldAll to prevent Mathematica from automatically ordering the output. We use LaTeX macros which make their implementation easier. We translated four families of functions into LaTeX after rearranging the expressions. We use string replacement rules on the output with StringReplace. We use the following string rules to format computable Mathematica expressions: those for very-well-poised hypergeometric series, for QHypergeometricPFQ, and for QPh and QPhI. In our Wolfram Language implementation, we ultimately apply TeXForm followed by ToString. We will conclude our presentation by giving some detailed examples with PDF output.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Noah Schulman |
| **Academic Institution:** | College of William and Mary |
| **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Pursue a career in the technology industry after earning a master's degree in computer science |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Information Access Division, Multimodal Information Group |
| **NIST Research Advisor:** | Jim Horan, Haiying Guan |
| **Title of Talk:** | Evaluating Generative AI Audio Deepfake Tools |

**Abstract:**

The objective of the project is to perform a survey on the modern open source audio deepfake tools, test and understand the limitations and advantages of them, and explore their potential use cases in conjunction with other contemporary AI technologies such as large language models (LLMs). An audio deepfake involves leveraging artificial intelligence and machine learning techniques to generate synthetic audio content that convincingly replicates the voice of a specific individual. While this technology holds promising applications, such as enabling individuals who have lost their voices to communicate naturally, it also poses risks, including the potential for malicious use and the spread of misinformation by imitating public figures. As advancements in AI and computing continue, audio deepfake tools have become more accessible, user-friendly, and capable of producing high-quality results. This project encompasses a comprehensive evaluation of existing open source audio deepfake tools, analyzing their common techniques, usability, quality, and implications. This evaluation involves modifying these tools' training datasets and textual inputs to gain a comprehensive understanding of their capabilities and limitations. Furthermore, it explores the potential benefits and challenges of combining audio deepfake technology with other popular AI tools, such as large language models, to understand their combined power, accessibility, and usability for the general public.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Kaylin Yeoh | |
| **Academic Institution:** Carnegie Mellon University | **Major:** Information Systems |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Graduate School/Consulting/Product Management/Data Analytics |
| **NIST Laboratory, Division, and Group:** | Information Technology Lab, Information Access Division, Visualization and Usability Group |
| **NIST Research Advisor:** | Afzal Godil |
| **Title of Talk:** | An Evaluation of Synthetic Data Generation Methods for Tabular Data |

**Abstract:**

Synthetic data is a fairly new and hot topic in the artificial intelligence world. It can be defined as artificially annotated information generated by computer algorithms or simulations. The use of synthetic data is gaining wide acceptance from all over the world as it serves many benefits over real-world data, including: increased security and privacy for sensitive data, cost-effectiveness, customizability for testing purposes, faster data generation, resolving imbalance datasets, etc. However, synthetic data generation also comes with some challenges. Since this is still a relatively fresh topic, researchers are still looking to find ways to overcome problems with lack of accuracy, overlooked outliers, real data dependency, and more, so that synthetic data will be reliable and used more frequently in real world settings.

With the variety of datasets and numerous ways of generating synthetic data, this paper will explore 3 different types of datasets (unbalanced, balanced, mixed) and evaluate the outcomes of synthetically generated data using selected models in 3 areas: statistical models, generative adversarial networks (GANS), and neural networks. Evaluation of synthetic data generated by the selected models will be analyzed following 3 main criteria: 1) Machine Learning Usability, 2) Statistical Similarity, and 3) Privacy Conservation. This project will aim to identify the best models for distinct datasets, and provide a baseline evaluation method for all synthetically generated data.

# SURF Student Colloquium

NIST – Gaithersburg, MD
August 1-3, 2023

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|---|---|---|
| **Name:** Luke Zic | | |
| **Academic Institution:** Univeristy of Maryland, College Park | **Major:** Computer Science | |
| **Academic Standing (Sept. 2023):** | Sophomore | |
| **Future Plans (School/Career):** | Software Engineer | |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Information Access Division, Information Retrieval Group | |
| **NIST Research Advisor:** | George Awad | |
| **Title of Talk:** | Video Retrieval Evaluation Leaderboard Development | |

**Abstract:**

A 'competition leaderboard' is a leaderboard that presents results of submissions by research institutions in reference to a challenge outlined by the publisher of the leaderboard. In this case, the leaderboard will present metrics that pertain to a TREC Video Retrieval Evaluation (TRECVID) competition, hosted by NIST. The goal of the leaderboard is to create healthy competition between research institutions for the advancement of our Artificial Intelligence, as applied in video understanding knowledge and techniques.

The goal of my project is to create a comprehensive 'competition leaderboard' that will take in, evaluate, score and present the results of a TRECVID competition outlined by NIST researchers. The leaderboard will consist of a multitude of parts: joining form, submission form, task specification form, and the leaderboard itself. Every step of the way, data will need to be configured and submissions scored to get the metrics and information requested by NIST. NIST researchers will have the power to modify which metrics are presented on the leaderboard, and thus control what metrics are evaluated from the TRECVID runs. Each form, including the leaderboard, will be run on a NIST external server for any valid institution to participate and submit their results.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


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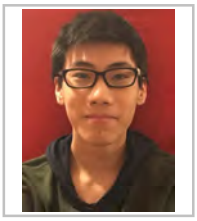
|---|---|
| **Name:** | Marilyn Nguyen |
| **Academic Institution:** | University of Maryland, Baltimore County |
| **Major:** | Information Systems |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Finish my Bachelor's Degree and pursue a Master's Degree in Information Systems |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Computer Security Division |
| **NIST Research Advisor:** | Ketan Mehta |
| **Title of Talk:** | Implementations of Mobile Driver's Licenses and Everyday Documents |



**Abstract:**

Today's society is continually expanding the use of technology in our everyday lives. This includes the increasing use of digital identity documents and other personally identifiable information. These documents range from mobile driver's licenses to digital plane tickets, digital payment options, and many other document classifications. The use of mobile devices has numerous benefits such as reducing costs, enhancing user experiences, and allowing a platform for countless documents to be easily stored. Instead of using physical wallets and purses that are cumbersome to carry and easy to misplace, we are transitioning to convenient and more secure storage of digital documents on mobile devices, generally called mobile documents. Digital wallets also offer a stronger sense of security as the threat of losing or having your documents get stolen is reduced. NIST has been working on producing standards for these mobile documents to ensure the safety and security of users' information through extensive authentication, verification, identity proofing, and identity assurance. Currently, we are addressing the importance of using digital identity documents securely and responsibly on mobile devices. With the use of standardized Identity Assurance Levels (IAL) and Authentication Assurance Levels (AAL), users and other relying parties can be assured of their information's privacy and security, protecting against fraud, unauthorized use of documents, and other threats. In addition, NIST is researching additional capabilities and guidelines to make utilizing mobile documents more efficient and effective in people's daily lives. My responsibility in this project is to research other methods that mobile documents can be utilized and determine various requirements for each method. In this research project, our essential goal is to discover ways we can implement the mobile driver's licenses' standards and data models into mobile Personal Identity Verification (PIV) cards and FAA Pilot Licenses. To do this, we are creating namespaces and collecting essential data elements required for the PIV cards and FAA Pilot Licenses, and researching the standards listing how these documents can be secured and authenticated when in use.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Alex Dai | |
| **Academic Institution:** University of Maryland - College Park | **Major:** Computer Science |
| **Academic Standing (Sept. 2023):** | College Senior Student |
| **Future Plans (School/Career):** | Graduate and work on a master's degree after obtaining a job |
| **NIST Laboratory, Division, and Group:** | ITL - Computer Security Division - Secure Systems and Applications Group |
| **NIST Research Advisor:** | Ketan Mehta |
| **Title of Talk:** | Exploring Suitable Structures to Store mDoc Field Data. |


**Abstract:**

Currently, our group is working on an alternative form of verifiable identification. We predict that, in the future, physical IDs may eventually grow obsolete, thus an existing standardized digital alternative would be convenient if society decides to shift identification to a digital medium. So far, the group has constructed a functional application (referred to as the "mDL application") that stores, verifies, and reads driving license data, in a document format of the name "mDL" (Mobile Driving License). An mDL is one of many mobile documents (mDocs) that the team wishes to cover with the mDL application. The same standard can be leveraged to support multiple documents.

As of now, the application is only calibrated to the mDL format, and my objective over the summer is to come up with a method to store multiple document formats. While there are many solutions available that would satisfy the objective, each solution comes with varying degrees of accessibility and, conversely, security.

Once a suitable solution is discovered and agreed upon by members of the mDL application team, I would like to attempt to implement the solution as a branch of the mDL application, in hopes that my work can be of contribution to the team.

If successful, my contribution could aid in the creation of the mDL application and encourage the creation of multiple mDoc types.

# SURF Student Colloquium

NIST – Gaithersburg, MD
August 1-3, 2023

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| **Name:** Brian Chen | | | |
| **Academic Institution:** | Towson University | **Major:** | Computer Science Cyber Operations |
| **Academic Standing (Sept. 2023):** | Senior / 4th year | | |
| **Future Plans (School/Career):** | Complete Cyber Operations track in Computer Science at Towson University / CyberCorps SFS / Master of Science: Specialization in Machine Learning | | |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory / Computer Security Division / Security Engineering and Risk Management (773.04) | | |
| **NIST Research Advisor:** | Jim Foti | | |
| **Title of Talk:** | Graph Database for NIST Cybersecurity Publication Citation Relationships | | |


**Abstract:**

NIST develops and maintains cybersecurity standards and guidelines that are critical resources used by Federal Government agencies to secure information and information systems. They are widely used by consumers and in private sector enterprises, notably in the financial sector and other critical infrastructures. At present, NIST manages more than 190 of these cybersecurity standards and guidelines, which have many interrelationships that must be understood by NIST staff and external users. Maintaining this complex publication portfolio requires both a simpler and more robust strategy for organizing bibliographic information.

The purpose of this project is to use graph database technology to model the citation relationships amongst NIST's current cybersecurity standards and guidelines. The goal is to improve publication life cycle management and provide multiple audiences with new tools for visualizing publication interrelationships.

In this study, a graph model and database using the Neo4j application examines NIST's collection of cybersecurity standards, including Federal Information Processing Standards (FIPS) and Special Publications (SP) 800-series guidelines and recommendations. Neo4j's data modeling utilizes informative and detailed labels, properties, and relationships to easily identify NIST publications that need to be updated or withdrawn, as well as other publications that will be impacted by those changes.

This tool can help advanced users and those with limited cybersecurity knowledge to better conceptualize and follow the many relationships among NIST's cybersecurity publications.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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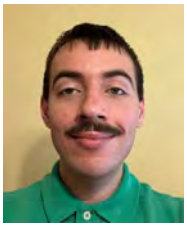
|---|---|
| **Name:** | Jayden Crosby |
| **Academic Institution:** | North Carolina A&T University |
| **Major:** | Computer Engineering |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | I plan to have a career in Cybersecurity |
| **NIST Laboratory, Division, and Group:** | Computer security |
| **NIST Research Advisor:** | Jeffery Voas |
| **Title of Talk:** | Integrating a Chat-bot for NIST |


**Abstract:**

My first Summer task was to: (1) learn how chatbots work, and (2) create a simple chatbot that could read official NIST documents. The main purpose of this task was to predict/discover the difficulty in creating a "real chatbot" in the future that could be added to the NIST.gov site to help users find cybersecurity information from NIST's numerous cybersecurity publications. The secondary purpose of this task was that my mentor wanted me to learn about chatbot technology before I return to college. This task was straightforward for the most part; I was able to find a site where I could create a chatbot without writing any additional code. I used the tool Engati (https://www.engati.com/blog/build-a-chatbot-in-10-minutes) from a list of alternatives 1 . I trained the bot by uploading two NIST publications into it, "Users are not stupid: Six cyber security pitfalls overturned" and "Cybersecurity Framework Profile for Liquefied Natural Gas." When testing the bot, I asked it multiple questions about cybersecurity based on the two documents, but the bot was so simple that it was only able to recite parts of the 2 publications that had the keywords to the question I asked. The bot should yield far better results: (1) if more documents were fed into it, and (2) if code had been written for it (but my free temporary license to Engati expired before I could do that). I am now beginning to use public chatbots (e.g., chatGPT) as well as other search engines to retrieve information concerning the energy consumption of various IT technologies, including cybersecurity approaches, for my final report in August.


1
https://www.tidio.com/blog/how-to-create-a-chatbot-for-a-website/
https://www.appypie.com/chatbot/builder



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NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Francis Durso

**Academic Institution:** Johns Hopkins University | **Major:** Computer Science

**Academic Standing (Sept. 2023):** Full-Time student, Senior

**Future Plans (School/Career):** Software Developer / AI Engineering / 5th Year Masters

**NIST Laboratory, Division, and Group:** Information Technology Laboratory, Computer Security Division

**NIST Research Advisor:** Dr. Raunak and Dr. Kuhn


**Title of Talk:** A Combinatorial Approach to Explainable AI

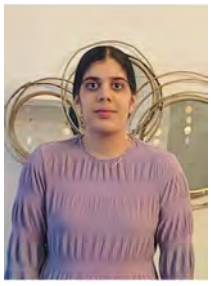

**Abstract:**

Recent advances in Artificial Intelligence and Machine Learning (AI/ML) systems have been extraordinary. These systems not only produce remarkably accurate outputs, they even outpace human performance in many cases. The level of accuracy, however, appears to be inversely related to the explainability and interpretability of these systems, which in turn can make them lack trustworthiness.

Combinatorial methods have been shown to be highly successful in software testing, discovering both well-hidden faults as well as their origins. Combinatorial testing systematically and efficiently covers the input space of a system by utilizing n-way interactions (n=1,2,3, etc.), known as covering arrays, amongst the parameter values.

The combinatorial fault location algorithm can be utilized to also provide insights into the factors influencing a machine learning algorithm's classification decision. For example, with a set of input value combinations that a binary classification based ML model puts in one class (class members) vs. input value combinations that result in a different class (non-class members), it is possible to determine which value interactions occur solely or at a far greater rate within one set than the other. This can lead to identifying which set of input value combinations are determining, or at least significantly influencing, the classification decision. This approach not only can provide insights into what a classifying ML algorithm has learned, it can also provide contrastive, causal, and counterfactual explanations in some cases, which have been shown to be considered highly trustworthy by human users.

Based on the above ideas, we have been developing a command-line tool which accepts a class and non-class file, and returns all 1, 2, and 3-way combinations of variable values which appear in one file or another at a frequency greater than a user-chosen threshold. Additional information is also returned about each file and their overlaps, as well as graphs depicting the combinations returned. Continuing in this SURF project, we are enhancing this approach and developing a graphical tool with more features that can help towards explaining the inner workings of a black box AI/ML system.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

**Name:** Navya Gautam

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

**Major:** Computer Science and Mathematics

**Academic Standing (Sept. 2023):** Senior

**Future Plans (School/Career):** I plan to pursue a career in computer science and cybersecurity.

**NIST Laboratory, Division, and Group:** Information Technology Laboratory (ITL), Computer Security Division, Security Engineering and Risk Management Group

**NIST Research Advisor:** Hung Trinh and Kate Schroeder

**Title of Talk:** Creating an Enriched Cybersecurity Risk Dataset with Visualizations to Analyze and Evaluate Cyber Risk Incidents

**Abstract:**
In today's digital age, the importance of cybersecurity cannot be overstated. Currently, the amount of available information and data relevant to cybersecurity risk analytics does not match this ever-expanding importance. Our team at NIST is continuously working to establish widely available and standardized methods and tools to identify, evaluate, analyze, and mitigate cyber incidents.

This project includes creating a centralized database that pulls and effectively organizes cybersecurity incident information from a variety of available sources. To accomplish this, we leverage ethical web scraping, Python, and R. This database will be used to support the cyber incidents data analytics repository (CIDAR). The original data sources come from organizations with different goals reflected in the way they collect and store their cybersecurity information. Some of the data is common among these sources, so we need an automated way to eliminate exact syntactic redundancies and redundancies that are less immediately obvious. This includes using Natural Language Processing for fuzzy string matching to detect common entries in different databases and fitting a logistic regression model that helps us predict whether two entries are duplicate. Once these duplicate entries are detected, they must be removed based on an established identifier while one representative event remains.

Since it can be difficult to view trends and relationships between cyber incidents in a tabular format, we utilize Neo4j to create our graph database using our enriched dataset to view relationships among event nodes.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|
| **Name:** Anthony Malysz | | |
| **Academic Institution:** Harvard College | | **Major:** Mathematics & Computer Science |
| **Academic Standing (Sept. 2023):** | Junior, Class of 2025 | |
| **Future Plans (School/Career):** | Currently exploring Cybersecurity (pentester/researcher in government/corporate work); may pursue PhD in the future if work demands it. | |
| **NIST Laboratory, Division, and Group:** | Information Technology Lab (ITL), Computer Security Division (CSD), Secure Components and Mechanisms Group (773.02) | |
| **NIST Research Advisor:** | A.J. Stein | |
| **Title of Talk:** | "Next Generation Policy-as-Code" | |


**Abstract:**

IT governance and information security policies are often complex to formulate, and even more complex to implement. Technical management and organization executives draft policy language with the intent to inform all employees---not necessarily engineers, let alone the computers themselves---who must actualize said policies. After policy language is drafted, expert technical staff are needed to implement the policy to their respective technical domains, such as network and security administration of Linux operating systems. Oftentimes, rigorous information security programs require additional impartial, third-party experts to come and assess the implementation and review its readiness for production use separate of those that wrote the policy and implemented the systems to support it.

In short, even minor policy changes require significant trickle-down efforts by skilled employees in high-demand sectors of industry that are difficult to employ and retain. It would be ideal to have software read and interpret these plain-English policy documents instead, providing code in the appropriate domains to implement and assess them. In this project, we aim to explore this research space with the following approach:

1.) Review the current state of software and machine learning models to convert policy documents to Linux system network and security administration functions in a semi-automated or completely automated fashion.
2.) Build a naive prototype with a visual interface to handle "formatted" human-friendly policy documents and convert them into PCAP expressions now (and eBPF in the long-term) for a novel Policy-as-Code approach to manage network and security functions for modern Linux operating systems.
3.) Publicize this repository as open-source project for the long-term goal of integrating more sophisticated machine-learning models in translating English sentences, integrating existing open-source projects into NGPaC for added functionality, searching for specialized data with which to train and test these models with, and more.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** John Guerrerio | |
| **Academic Institution:** Dartmouth College | **Major:** Computer Science |
| **Academic Standing (Sept. 2022):** | Sophomore |
| **Future Plans (School/Career):** | Graduate School |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Software and Systems Division, Software Quality Group |
| **NIST Research Advisor:** | Dr. Irena Bojanova |
| **Title of Talk:** | Understanding Memory-Related CWE Entries with Bugs Framework |

**Abstract:**

The Common Weakness Enumeration (CWE) is the most widely used repository of software and hardware weaknesses [1]. The CWE lists types of weaknesses, but it lacks an explicit conceptual model of their underlying role in vulnerabilities. In this work, we use the Bugs Framework (BF), an orthogonal, language independent taxonomy for classifying software bugs and weaknesses, to clarify and supplement the CWE entries [2]. We first verify and improve the set of BF operation and final error mappings from the CWEs to the BF Memory Bugs class types originally produced in [3]. We then identify BF weaknesses (cause-operation-consequence triples), or BF chains of weaknesses. To accomplish this, we analyze the CWE descriptions, extended descriptions, corresponding Common Vulnerabilities and Exposures (CVE) [4], as defined by the National Vulnerability Database (NVD) [5], and other associated data. We identify CWEs with corresponding BF weaknesses or chains and examine their semantic similarity scores (generated by SpaCy) [6]. The latter allows us to investigate BF's ability to capture similarities between CWEs. Our work makes explicit the tacit model of the CWEs, as well as suggests that BF has the capability of identifying areas where the CWE List could be improved. These initial mappings and additional ones involving other BF class types would allow BF and CWE to leverage each other's advances and provide users a bridge between the two. Future work could utilize these mappings in the development of semantic models of the CWEs and CVEs.

[1] MITRE, Common Weaknesses Enumeration (CWE), https://cwe.mitre.org/.
[2] NIST, The Bugs Framework, https://samate.nist.gov/BF/.
[3] I. Bojanova and C. Eduardo Galhardo, "Classifying Memory Bugs Using Bugs Framework Approach," 2021 IEEE 45th Annual Computers, Software, and Applications Conference (COMPSAC, 2021, pp. 1157-1164, doi: 10.1109/COMPSAC51774.2021.00159).
[4] MITRE, Common Vulnerabilities and Exposures (CVE), https://cve.mitre.org/.
[5] NVD, National Vulnerability Database (NVD), https://nvd.nist.gov.
[6] M. Honnibal and I. Montani, "Natural Language Understanding with Bloom Embeddings, Convolutional Neural Networks and Incremental Parsing," unpublished, 2017, https://spacy.io/.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


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|---|---|
| **Name:** | Zach Benton |
| **Academic Institution:** | Stanford University |
| **Major:** | Math |
| **Academic Standing (Sept. 2022):** | Junior (3rd year) |
| **Future Plans (School/Career):** | Graduate School in Computer Science |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory / Software and Systems Division / Information Systems Group |
| **NIST Research Advisor:** | Antonio Cardone |


**Title of Talk:** Crowdsourcing Testing Images for CNN-Based Solutions to Image Texture Directionality


**Abstract:**

Texture directionality is a salient property of materials, relevant in a number of scientific fields. For example, the direction of extracellular collagen bundles has been found to correlate to the dissemination of
cancer cells, and the direction of wood grain determines the strength of wood as a construction material. Recently, my NIST supervisors have developed a convolutional neural network (CNN) that can determine texture directionality. A huge amount of real-life data is necessary to properly test the CNN; so far the CNN
has only been quantitatively tested on synthetic data. To collect the hundreds of thousands of real-life images necessary to test the CNN, I have built a globally accessible database to house images and their texture directionality annotations. I coded the website on Java, using Eclipse as my integrated development environment.

The database uses MongoDB to store image metadata—including image annotations, owner, name, keywords, and more. MongoDB includes an abundance of filter functionality, so I also created a simple search service on the website, allowing users to search the image database by owner and image name. I intend to expand this feature to include a more robust collection of search fields.

I also created a directionality annotation software in JavaScript that enables users to annotate the database's images while on the website. The software splits an image into a grid of rectangular tiles, then it allows the user to specify the directionality, in degrees, of the image's texture within each tile. There are
many features I intend to add to this image annotation software, including further customization of tile locations and spacing, a way for users to indicate their confidence in the direction they selected for each tile, and potentially allowing users to select multiple directions for each tile.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Vidhata Jayaraman | |
| **Academic Institution:** University of Illinois Urbana-Champaign | **Major:** Electrical Engineering |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Ph.D and then a career in research |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Software and Systems Division |
| **NIST Research Advisor:** | Alden Dima |
| **Title of Talk:** | Surprising Sentences |

**Abstract:**

It is a common occurrence in text analysis that one wants to identify surprising sentences in a dataset. The contemporary approach to such a task would be to train or fine-tune a large language model (LLM) to identify surprising sentences. However, in low resource domains, there is often not enough data, resources, or time to allocate to training such a model so other approaches are necessary. One such approach is to use embeddings to embed the sentences, dimensionally reduce them and then by treating each feature of the dimensionally reduced embeddings as a variable, calculate surprisal values for each sentence. Three major dimensionality reduction methods are proposed: Principal Component Analysis (PCA), Independent Component Analysis (ICA), and Kernel Principal Component Analysis (KPCA). These methods were compared to an older method using Term Frequency Inverse Document Frequency (TF-IDF) and a contemporary fine-tuned GPT-2 model for identifying surprising sentences. I find that all methods succeed in finding probable surprising sentences, however we find that the proposed dimensionality reduction methods along with GPT-2 better capture sentence semantics than the older TF-IDF method. This means that the newer methods are better able to identify sentences that contain truly strange meaning rather than just differences in sentence structure. However, for large text data, inverse term frequency is still a very good measure of how surprising a sentence is, so the TF-IDF does seem to generally function "better" than the dimensionality reduction methods. Furthermore, comparing the results of the TF-IDF and dimensionality reduction methods to the fine-tuned GPT-2 model, while the dimensionality reduction methods seem to generally be consistent with the GPT-2 model, the TF-IDF method is consistently the most similar in ranking to the GPT-2 model. However, fine-tuning a GPT-2 model takes a lot of time and resources so the general relationship between the dimensionality reduction methods and the GPT-2 methods indicate that these dimensionality reduction methods may still be very usable.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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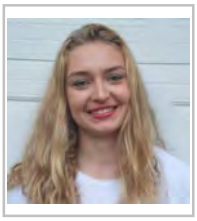
|---|---|
| **Name:** | Ishaan Bhardvaj |
| **Academic Institution:** | University of Maryland |
| **Major:** | Computer Science and Economics |
| **Academic Standing (Sept. 2023):** | Sophmore |
| **Future Plans (School/Career):** | Graduate School |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Divison 775 Cyber Infastructure Group |
| **NIST Research Advisor:** | Ya-Shian Li-Baboud |
| **Title of Talk:** | Impact of Weather Parameters on Path and Clock Delay in Quantum Networks |


**Abstract:**

The operation of a metropolitan-scale quantum network relies on the near simultaneous arrival of photons within 10 picoseconds. Weather conditions including temperature, humidity, cloud cover, and wind speed introduce fluctuations and noise in path delay and time synchronization. This project aims to create a methodology to understand and rank the significance of available weather factors on optical fiber path delay variability. A secondary goal is to evaluate the feasibility of using historical weather data to train a predictive model for path delay. The path delay between a NIST-UMD link was gathered using a white rabbit switch . Weather data was gathered using the OpenWeatherMap and TomorrowIo weather APIs. Correlation analysis was conducted to rank weather factors that impact path delay. The analysis revealed that temperature and humidity were the most significant factors influencing path delay prediction. Additionally, wind speeds exceeding 8 meters per second were shown to have a noticeable impact on path delay. Based on these findings, a random forest algorithm was trained to predict path delay, achieving a MAPE of under 10% within the same dataset. This study demonstrates the importance of considering weather parameters for accurate prediction of path delay in quantum networks. They highlight the complex, interconnected nature of weather parameters and time stability. In the future, we plan to develop a comprehensive weather querying system that covers the entire NIST-UMD testbed for a more holistic analysis of weather. Further, we hope to implement weather forecasting into our model so that it is more robust and works in real time.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Kathryn Butziger

**Academic Institution:** Worcester Polytechnic Institute | **Major:** Computer Science

**Academic Standing (Sept. 2023):** Senior


**Future Plans (School/Career):** Pursue graduate school

**NIST Laboratory, Division, and Group:** ITL, Software and Systems Division, Information Systems Group

**NIST Research Advisor:** Dr. Peter Bajscy

**Title of Talk:** Comparison of AI Model Attribution Methods


**Abstract:**

NIST has been exploring methods that explain encodings of trojans in AI models. The AI community has published several approaches to explain and interpret AI model predictions. The approaches range from designing attribution methods (e.g., identify importance of pixels in computer vision (CV) related AI-modeling tasks) to analyzing classes of machine learning and artificial intelligence (AI) supervised models. The objective of this project is to understand (1) the reliability of multiple implementations of existing attribution methods (i.e., reproducibility of attribution maps as a function of implementation frameworks), (2) the sensitivity of attribution maps to their AI model architectures and algorithmic parameters, and (3) the applicability of the attribution methods to detecting trojans in poisoned images.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Carina Carino

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

**Academic Standing (Sept. 2023):** Recent Graduate

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

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

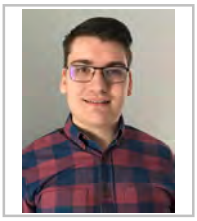
**NIST Research Advisor:** Dr. Joe Chalfoun, Dr. Adele Peskin


**Title of Talk:** Deep Learning-Based Viral Plaque Detection in Label-Free Phase Contrast Images


**Abstract:**

Viral vectors are widely used for gene therapy, vaccination, and cancer treatment due to their ability to effectively deliver foreign genetic materials into host cells. A thorough understanding of viral infectivity - the ability of a virus to invade, survive, and proliferate within host cells - is crucial to fully leverage the benefits of these vectors. Traditional plaque assays have been used to quantify viral infectivity but rely on staining techniques and manual inspection, introducing biases and limiting throughput. In this study, we propose a novel approach utilizing deep learning to semantically segment viral plaques from label-free phase contrast images. By automatically identifying and segmenting viral plaques, deep learning eliminates the need for staining and labor-intensive manual analysis.

Viral plaques display discernible differences in intensity and texture relative to their surroundings. As a result, we generated training set labels by applying a threshold to the intensity values, determined based on the mean and local standard deviation within the phase contrast images. These labels were subsequently used to train a 2D-UNet model, while a separate test set was used for inference. The resulting inferenced outputs were post-processed and evaluated for accuracy using the dice score. Initial test results demonstrated successful detection of viral plaques, indicating promising potential for an automatic label-free viral plaque detection method.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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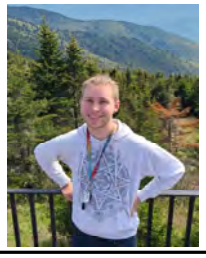
|---|---|
| **Name:** Ryan Trask | |
| **Academic Institution:** University of Maryland | **Major:** Biocomputational Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Finish my bachelor's at University of Maryland, and pursue graduate school afterwards. |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Software and Systems Division (775), Meniscus Effect Group |
| **NIST Research Advisor:** | Joe Chalfoun |
| **Title of Talk:** | Correction of the Meniscus Effect in Biological Samples with Convolution Neural Network Models. |


**Abstract:**

Phase contrast and bright field imaging of single cells in small well plates is distorted by adhesion of the liquid media to the walls of the well. This causes the microscopy light to be distributed unevenly across the media, making regions of the media unrecognizable by microcopy imaging technology. Therefore, large areas of these biological samples are rendered inaccurate for many image-based biological experiments. Many techniques exist to correct for the meniscus effect, such as QPI-Reference Image Matching and Ptychography. Nonetheless, these techniques are expensive or distort biological samples in other ways. This presents an opportunity for an image-to-image regression convolution neural network (CNN) to offer a competitive alternative to the literature techniques.

Collaborators in the Material Measurement Laboratory collected bright-field and phase contrast images of biological samples, with and without the meniscus effect. The meniscus effect was spread out, or removed, by placing a cover-slip over biological samples, between imaging the same sample two times. This provides us with the ground truth to train our CNN models. Providing multiple types of images or perspectives of the biological samples will allow the CNN models to learn more about correcting the meniscus effect. Image registration was conducted between phase contrast and bright-field image data due to translational differences caused by image stitching. The neural network architecture chosen is the U-Net architecture, modified for image-to-image regression from the normal semantic segmentation network, due to its better performance over a ResNet architecture on this dataset. Loss is measured by the Root Mean Square Error (RMSE) pixel difference between pixel values with and without meniscus. Several CNNs have been trained to correct the meniscus effect on a separate dataset which was collected in the same manner as the data used to train the CNN models. These results are quantified by calculating the RMSE between the model's correction of the meniscus effect and that of the cover-slip technique.



# SURF Student Colloquium

NIST – Gaithersburg, MD
August 1-3, 2023


**Name:** Stanley “Troy” Conklin

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

**Academic Standing**
**(Sept. 2023):** Senior

**Future Plans**
**(School/Career):** Work in industry with computer vision and / or graphics, then pursue grad school.

**NIST Laboratory,**
**Division, and Group:** Information Technology Laboratory, Software and Systems Division, Additive Manufacturing

**NIST Research**
**Advisor:** Timothy Blattner

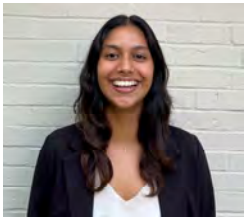

**Title of Talk:** Creating Abstractions for Real-time Image Processing


**Abstract:**

Additive manufacturing, or 3D printing, is the process of creating 3D objects by successively laying down layers of material. Power bed fusion is a type of additive manufacturing which uses a laser to melt layers of metal powder, producing a 3D object. In the process, some sparks may eject molten material from the object and create a defect. These events occur very quickly, and so detecting these events in real-time requires images to be captured and processed at 10,000 fps. The goal of this project is to interface with a high-frame rate camera and create useful abstractions to guarantee real-time performance.

We are able to achieve this performance using Hedgehog. Hedgehog is a C++ library created at NIST which allows for coarse-grained parallelism. Tasks in a program are represented as nodes in a graph and the data flowing between tasks are the edges between them. Each task is physically bound to its own thread, allowing for the tasks to run in parallel. We use Hedgehog to define an abstraction for grabbing and processing frames and offset slower tasks to run in “soft real-time”. Importantly, this abstraction comes with guarantees of real-time performance.

Finally, we implement the abstraction for cameras which support the GenICam API – a standard interface for getting and setting information from a camera. To test this abstraction, we use a GigaSens camera that implements the GenICam API. We are able to verify that our setup captures frames, sends frames to memory, as well as processes images with OpenCV’s findContours function in real-time at our target rate of 10,000 fps.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Sonika Sharma | |
| **Academic Institution:** University of Delaware | **Major:** Computer Science |
| **Academic Standing (Sept. 2023):** | Rising Senior |
| **Future Plans (School/Career):** | I will work for the governement and earn a Masters degree |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Software and Systems Division, Software Quality Group |
| **NIST Research Advisor:** | Dr. Paul E. Black |
| **Title of Talk:** | Confirm That 25 747 New Programs Can Replace the 32 003 Programs of the Old C# Test Suite |

**Abstract:**

Software assurance is crucial for the reliability, functionality, and security of computers in society. Even when software is built well, static analysis and testing are vital to gain assurance about exploitable vulnerabilities. NIST's Vulnerability Test Suite Generator (VTSG) creates tests for static analyzers. This March NIST scientists used VTSG to create a new test suite of 25 747 C# programs. This new test suite improves upon the existing C# test suite developed seven years ago by correcting mistakes and removing unnecessary test cases. This project is to validate the new test suite so it can replace the existing one. Validation comprises compiling and executing all of the programs one at a time and confirming that each one presents its intended vulnerability. To start, we had to write hundreds of lines of Linux commands, including grep, find, Perl, wc, and Bash, to validate and prepare the test suite. The existing programs are test suite 105 in the SAMATE Software Assurance Reference Dataset (SARD) https://samate.nist.gov/SARD/ To update test suite 105, we mapped new files to existing files and confirmed that the new version will preserve information content. By enabling more reliable identification of security flaws and design weaknesses in software, we strengthen the foundation of dependable computer technology.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Saahil Singh |
| **Academic Institution:** | University of Maryland - College Park |
| **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Software Engineering with an AI/ML focus |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Software and Systems Division, Cyber Infrastructure Group |
| **NIST Research Advisor:** | Sarala Padi |
| **Title of Talk:** | Mapping Categorical Emotions and Dimensional Attributes from Text Data to Sentiment Scores |


**Abstract:**

Analyzing human behavior in the real world is a complex task that requires specialized methods such as emotion recognition and sentiment analysis. While sentiment analysis focuses on identifying positive or negative markers, emotion analysis provides a broader understanding of human emotions and sensitivities. Building an emotion recognition model is a challenging endeavor that can be made simpler by incorporating sentiment scores as a guide. To do this, we must first generate sentiment scores from categorical emotions and dimensional attributes. Categorical emotions include joy, frustration, sadness, and other complex or simple emotions, while dimensional attributes refer to values on a scale that represent the intensity and characteristics of emotions, such as valence (the positivity or negativity of an emotion), arousal (the intensity of an emotion), and dominance (the power expressed by an emotion). These two methods of labeling emotions offer a unique perspective on the emotional content of the data but directly mapping them to sentiment scores can be difficult. Our goal is to build and evaluate models that can effectively transition categorical or dimensional labels to sentiment labels while addressing any inaccuracies or discrepancies in traditional methods. This research explores machine learning models and mapping mechanisms to generate sentiment scores, with a focus on two benchmark datasets called IEMOCAP and MELD. By addressing inconsistencies and designing an accurate model, we ultimately aim to construct a comprehensive understanding of emotion recognition models from text data.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Max Filliben

**Academic Institution:** University of Maryland-College Park | **Major:** Mathematics

**Academic Standing (Sept. 2023):** Junior

**Future Plans (School/Career):** Graduate school in Applied Mathematics or Statistics

**NIST Laboratory, Division, and Group:** Information Technology Laboratory, Statistical Engineering Division, Statistical Design, Analysis, and Modeling Group

**NIST Research Advisor:** Dr. Dennis Leber, William Guthrie


**Title of Talk:** Web-based Statistical Tools for Radionuclidic SRMs


**Abstract:**

Standard Reference Materials (SRMs) are an important product that NIST produces. Laboratories across campus are dedicated to the development and precise measurement of reference materials ranging from chemical solvents to peanut butter. These materials are used by industry for a variety of reasons including adherence to environmental regulations and instrument calibration.

Many SRMs are created more than once, so standardized processes are important. The purview of these processes covers both the manufacturing of the material and the reduction of measurements to values and associated uncertainties for physical or chemical properties of interest.

This summer, we created versatile statistical tools that aid in the analyses of radionuclidic SRMs. In doing so, we simulated data based on SRM 4330c (Plutonium-239) and other radionuclidic SRMs and implemented a series of statistical tests tailored to the SRM certification process. We found that many of these tests, when compared to the original statistical analysis, were more reliable and conclusive, eliminating hidden biases and correlations that impede their statistical efficacy and validity.

Two key characteristics of SRM data analysis are their reproducibility and ease-of-use. We coded the statistical tests into an R-based web application that generates the user-selected analyses and graphics with the input of a data file. The application also autogenerates a report using R Markdown that includes all relevant information documenting the data analysis of the SRM development. This application will serve to fill a gap in existing web-based statistical tools that are critical in SRM development.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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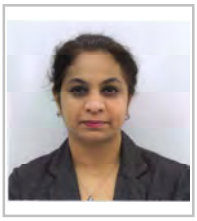
|---|---|
| **Name:** David Sadek | |
| **Academic Institution:** University of Maryland-Baltimore County | **Major:** Computer Science |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Software Engineer |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Statistical Engineering Division, Statistical Design, Analysis, and Modeling Group |
| **NIST Research Advisor:** | Dr. Adam Pintar |
| **Title of Talk:** | Errors in Variables Regression Models |

**Abstract:**

For the 2023 SURF Internship, I am building a frontend graphical user interface for the purpose of running backend statistical computations. This interface is built through Shiny for Python, which creates a browser-based interface to run said computations. The interface is aimed to be user-friendly and interactive. The statistical computation is fitting errors in variables regression models (also known as measurement error models). These models assume that there are errors in the measurements of both the dependent and independent variables. In contrast, ordinary least-squares regression assumes only errors in the measurement of the dependent variable.

Our motivating application is nanoparticle measurements, which are important to many areas of science including nanomedicine and determining the harmful effects of plastic pollution. For example, lipid nanoparticles act as the delivery system for the COVID-19 vaccine, and plastic nanoparticles that degrade from larger plastic trash sorb heavy metals toxins. In both applications, the way in which substances (vaccine or toxin) adhere to nanoparticles is crucial to understand.

Our benchmark data set contains measurements of polystyrene spheres. The particles were loaded with fluorophores, dispersed into a fluid, and injected into a stair step structure. They were then optically imaged to simultaneously measure fluorescence intensity (dependent variable) and size (independent variable). Location within the stair step structure informs size. Transmission electron microscopy measurements of a separate sample of particles is used to assess the magnitude of errors in the star step size measurements. The presentation will conclude with a live demonstration of the software using the polystyrene sphere data set.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

| | |
|---|---|
| **Name:** Femina Amoo | |
| **Academic Institution:** Montgomery college, Germantown, MD | **Major:** Cybersecurity |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Career in Cybersecurity |
| **NIST Laboratory, Division, and Group:** | Information Technology Laboratory, Applied Cybersecurity Division, NICE |
| **NIST Research Advisor:** | Danielle Santos |
| **Title of Talk:** | Evolution of cybersecurity education and workforce development |


**Abstract:**

According to the U.S. Department of Homeland Security, cybersecurity threats to critical infrastructure are among the most significant strategic risk for the nation.* As the information technology advanced by leaps and bounds in the previous decade, so have the capabilities of adversaries. Over the years, the United States has developed comprehensive plans to secure the country's critical infrastructure systems and assets. Among them have been the many initiatives, programs, competitions, and funding introduced within the field of cybersecurity in order to expand and create a more skilled, competitive, and diverse cybersecurity workforce. This sentiment can be seen in NICE's goals and plans since 2013, as conferences, presentations, and workshops had a few unifying goals: raising public awareness about cybersecurity, supporting formal cybersecurity education programs at all levels, and fostering a more diverse cybersecurity workforce.

The purpose of this research is to explore how cybersecurity education and workforce development has evolved over the years. One of the primary sources of the research will be the NICE website and conference materials dating back to 2013. Other sources such as websites of various government agencies, companies, and academic institutions will also be used. The following are some of the research questions that will be asked:

• How have the hiring practices changed in keeping with the changes in the past decade?

• How has the field of cybersecurity, from an educational and workforce standpoint, become more diverse over time?

 What is the role played by the NICE community?

 What is the role played by the NICE program office at NIST?

* https://www.dhs.gov/secure-cyberspace-and-critical-infrastructure

# Material Measurement Laboratory 2023

**Summer Undergraduate Research Fellowship (SURF) - 2023 Participants**

*(in the order of the Colloquium schedule)*

Material Measurement Laboratory (MML)

*George Sellers:* Using Electron Microscopy To Determine The Structure Of A Flexible Protein

*Grace Finch:* Replacing Sanger Sequencing with Next Generation Sequencing for Variant Allele Characterization

*Abigail Antonishek:* Quantitative and Qualitative Analysis of Lipid-Encapsulated mRNA

*Lily Min:* Digital PCR Assay Development for AAV Reference Materials

*Sophie Lipshutz:* How to protect cells during bioprinting

*Lukas Marple:* Advancing Metabolomics: How can we Improve Fecal Metabolite Extraction?

*Megan Nguyen:* Investigation of the Relationship Between Diet and the Human Gut Microbiome

*Maria Lindsey:* Comparison of Traditional In Vitro Viability Assays

*Jennifer Li:* Development of visualizations for the Genome In A Bottle data portal

*Jane Jou:* Detection of EML4-ALK Fusion Cancer Biomarker in Liquid Biopsy by EFIRM

*Walter Adamy:* Comparison of High-Rate and Quasi-Static Mechanical Testing for Aged and Unaged Single High Strength Fibers for Use in Body Armor Applications

*Ryan Punith:* Mechanical Testing of Heterogenous, Graded Impact Protection Materials

*Bradlee Rich:* Solving the worlds textile waste problem one blend at a time

*Max Mevorah:* Synthesis and Characterization of Metal-Impregnated Lewatit for Direct Air Capture (DAC)

*Tyler Hicks:* Exploration of Parameters for Carbon Nanotube Separations via Automated Fluorescence Titration

*Colin McCarragher:* Analysis of Polyzwitterion Solutions Using Dynamic Light Scattering

*Gabrielle Schumacher:* Liquid Crystal Elastomer Membranes for Enhanced Impact Resistance of 3D Structures

*Mia Merritt:* Study of Iron Oxide Nanoparticle Dynamics Based on Surface Functionalization for Magnetic Particle Imaging

*Muhammad Rafi:* Developing a spectral accurate solution to assess results for the Cahn-Hilliard benchmark

*Spencer Mattes:* Temperature and pressure dependence of dielectric spectra based on molecular dynamics simulations

*Nishwanth Gudibandla:* Understanding the Magnetic Properties of 2D Vanadium Diselenide with Density Functional Theory

*Aubrey Augustine:* Assessing Magnetic Levitation for Plastics Densimetry

*Leila Rose Clark (virtual):* Investigating Shear Induced Disentanglement Using the Slip-Link

*Leonardo Borchert:* Optimization of NanoCalorimetry Sensors using Finite Element Simulations

*Connor Davison:* Improving Toughness of CeriaBased Oxygen Ion Conductors

*Alison Hecht:* Exploration of diblock copolymer blend thin films to understand multicomponent system morphologies

*Evan Freeland:* Thickness Measurement of Gallium Phosphide Films on Silicon with Micro-X-Ray Fluorescence

*Arden Dombalagian:* Nanocalorimetry for Carbon Capture Materials Characterization

*Ryan Kim:* AELF multiagent machine learning to map transfer data

*Dennis Zhao:* Analyzing phase diagrams using machine learning

*Tristan Charles:* Utilizing Machine Learning to Analyze Carbon Dioxide Capture Efficiency

*John Marquart:* Similarity Metrics applied to Neural Networks: Examining how Material Properties are Learned

*Andrew Celi:* Integrated NIST Knowledge Website

*Jay Kannan:* Using the WIPP System for Imaging Cell-Virus Interactions

*Sheetal Padhi:* Containerized Tools for Image Processing and Analysis of Live Induced Pluripotent Stem Cells

*Carina Delcore:* An Investigation of Arginine-rich Antimicrobial Peptides and their Interactions with Lipid Membranes

*Jonah Oxman:* Characterizing Antibody Flexibility: 2D Codistribution Analysis of Disulfide Bond Reduction

*Sragvi Pattanaik:* Exploring the Role of Bacterial Motility in Evolutionary Mechanisms for Antimicrobial Resistance

*Kira Corning:* Generation of a Rapid GC-MS Library for Fire Debris Analysis and Ignitable Liquid Identifications

*Nikhila Narayana:* Compilation and Evaulation of Temperature Reference Points for the Alkali Metals

*Raine Antonio:* Bubble Trouble - Identification of Defect Sites in Glasses Using Optical Microscopy

*Jacob Blinkoff:* Modeling Chloride Diffusion in Concrete

*Sarah Lehrman:* Determining the yield stress and frequency dependence of printable thermoset composite resins

NIST MATERIAL MEASUREMENT LABORATORY

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


| | |
|---|---|
| **Name:** George Sellers | |
| **Academic Institution:** University of Maryland | **Major:** Biology: Neurobiology and Physiology |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Medical School, Clinical Researcher |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory, Biomolecular Measurement Division, Biomolecular Structure and Function Group |
| **NIST Research Advisor:** | Dr. Thomas Cleveland |


**Title of Talk:** Using Electron Microscopy To Determine The Structure Of A Flexible Protein


**Abstract:**

The purpose of the NIST Monoclonal Antibody Reference Material 8671 ("NISTmAb") is to serve as a standard for analytical methods used to study therapeutic proteins. The NISTmAb has been extensively characterized by different analytical techniques including UV-VIS spectroscopy, mass spectrometry, size exclusion chromatography (SEC), X-ray crystallography, NMR, and small-angle x-ray and neutron scattering (SAXS/SANS). Antibodies are flexible Y-shaped proteins consisting of rigid domains connected by a flexible hinge region in the middle of the protein. While it is generally possible to determine the structures of the isolated rigid domains, the distribution of flexible conformations they adopt is more difficult to experimentally determine. After using SEC to isolate monodisperse preparations of the NISTmAb and Aldolase, a control protein complex of comparable size, we performed cryo and negative stain electron microscopy on our samples. The conformational distribution of the NISTmAb was determined using a data processing workflow in CryoSPARC which included motion correction , CTF estimation, particle picking, 2D classification, and 3D variability analysis. This characterization of the NISTmAb conformational ensemble will provide additional context to aid in the interpretation of the large set of existing analytical data available for the NISTmAb. It also has the potential to yield greater understanding of antibody structure and function which could be useful in the development of protein based therapeutics in the future.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Grace Finch | |
| **Academic Institution:** Virginia Tech | **Major:** Biochemistry |
| **Academic Standing (Sept. 2023):** | Junior/Senior |
| **Future Plans (School/Career):** | After I finish my undergraduate degree I plan on pursuing a M.S. in Biochemistry |
| **NIST Laboratory, Division, and Group:** | MML, Division 645, Group 6 |
| **NIST Research Advisor:** | Becky Steffen |
| **Title of Talk:** | Replacing Sanger Sequencing with Next Generation Sequencing for Variant Allele Characterization |

**Abstract:**

For over 20 years the Applied Genetics Group (AGG) has provided the forensic DNA community with a free of charge service that enables sequencing of unusual, variant, and null short tandem repeat (STR) alleles found by members of the human identity testing community. Some of these alleles possess point mutations in primer binding sites leading to null alleles while others are "off-ladder" variants from commercial allelic ladders. Sequencing these unusual alleles helps to reveal the molecular basis for their variation. Sanger sequencing has traditionally been used at NIST for this service. However, this process has a low throughput capacity, making it time- and labor-intensive. The goal of this project was to develop a protocol for sequencing forensic DNA samples using Next Generation Sequencing (NGS), which is a newer, quicker, and more straight forward sequencing method, for the variant allele sequencing program. Testing was done to identify what parameters for polymerase chain reaction (PCR) worked best for sequencing including number of PCR cycles, amount of input DNA, and primer annealing temperatures. The ideal parameters were found to be 1 ng/ul input DNA with a 60ºC annealing temperature for 35 PCR cycles for most STR markers. However, there were some primer sets targeting the CODIS (COmbined DNA Index System) markers that had to be redesigned to yield more optimal results for NGS, including smaller amplicon sizes and functionality under the chosen parameters. Then the samples were sequenced using the Verogen MiSeq FGx Sequencing System and aligned to a reference sample from the GenBank sequence database from the National Center for Biotechnology Information (NCBI) to determine the genomic reason (single nucleotide polymorphism (SNP), insertion, or deletion) causing the variant allele.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Abigail Antonishek |
| **Academic Institution:** | Purdue University |
| **Major:** | Chemical Engineering |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Pursue Master's degree before working to address genetic disorders through gene therapy |
| **NIST Laboratory, Division, and Group:** | Materials Measurement Laboratory, Biomolecular Measurement Division, Bioanalytical Science Group |
| **NIST Research Advisor:** | Mark Lowenthal |
| **Title of Talk:** | Quantitative and Qualitative Analysis of Lipid-Encapsulated mRNA |


**Abstract:**

Messenger RNA (mRNA) is a form of RNA that is transcribed from genomic DNA and translated on a ribosome to produce proteins. Proteins are the building blocks of our bodies and play a critical role to our health. Recently, mRNA has emerged as a powerful therapeutic class for treatment and prevention of disease. One significant mRNA therapeutic in development is mRNA vaccines. An mRNA vaccine utilizes an mRNA strand, typically encased within a lipid nanoparticle for protection and delivery purposes, to initiate an immune response. The mRNA strand enters the patient's cells which then begin to produce the translated protein. This therapeutic enables the body to develop resistance to deadly diseases by introducing the body to foreign material, triggering an adaptive immune response so that the body can protect itself facing future encounters.

The quantity and quality of the mRNA in these vaccines and other drug products must be subjected to analytical scrutiny to ensure consistency, safety, and efficacy. Currently, there is no unbiased, traceable method for quantitative measurement of the mRNA contained within a lipid nanoparticle with high precision and accuracy. Other techniques, such as UV and fluorescence spectroscopy, droplet-digital polymerase chain reaction, and enzyme digestion with endonucleases, lack specificity, traceability, and calibration. Additionally, these approaches are unable to measure mRNA in situ meaning the LNP must first be lysed in order to access the enclosed mRNA for later measurement. However, an alternative method, acid hydrolysis, does both to completion.

This project seeks to demonstrate that in situ hydrolysis of a lipid nanoparticle-encapsulated mRNA therapeutic into constituent nucleobases and detection by liquid chromatography-mass spectrometry (LC-MS) is a precise and accurate method for quantitatively measuring mRNA. This is accomplished through acid hydrolysis of intact oligomers, a solution which is then analyzed by LC-MS in order to detect and quantify each nucleobase by its known molecular weight. The research team aims to optimize this method in order to prove it more robust, precise, and traceable than current methods. This research is applicable to accurately measuring mRNA concentrations in pharmaceutical products to support public safety and health.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Lily Min |
| **Academic Institution:** | University of Pennsylvania |
| **Major:** | Chemical Engineering and Biophysics |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Physician Scientist (MD-PhD) |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory, Biomolecular Measurement Division, Applied Genetics Group |
| **NIST Research Advisor:** | Megan Cleveland |
| **Title of Talk:** | Digital PCR Assay Development for AAV Reference Materials |

**Abstract:**

Gene therapy is a DNA modifying technique where therapeutic genes are introduced to the body to help treat a disease. The leading viral vector used for gene therapy is recombinant adeno-associated virus (rAAV). To calculate gene therapy dosages, quantitative PCR (qPCR) is often used. However, qPCR cannot calculate the absolute quantity of DNA in a sample without a reference material or calibrant. Due to the delicate nature of gene therapy, carefully calibrated reference materials for AAV are necessary for the standardization of gene therapy dosages across different laboratories. Unlike qPCR, digital PCR (dPCR) does not require a calibrant, making it ideal for measuring and certifying nucleic acid reference materials. Here, dPCR was used to develop assays that measure the quantity of DNA in a sample of AAV, using the serotype AAV2 as a test case. Various assays of primers and probes were pulled from literature or developed using online software such as Primer3Plus for a common region of AAV2 known as the ITR region, as well as for a CMV promoter and eGFP, which are present in this AAV material in place of a therapeutic gene. The ITR region is particularly difficult to develop assays for, due to the secondary structure which interferes with every step of the PCR process. While hypothetical annealing temperatures were provided from literature or online sources, they were optimized using gradient dPCR. The most accurate and efficient assays can be used to validate a future AAV reference material, which would be used to calibrate secondary reference materials for qPCR to ensure gene therapy doses are uniform throughout laboratories around the world.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Sophie Lipshutz |
| **Academic Institution:** | Georgetown University |
| **Major:** | Biology of Global Health |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate from Georgetown University and apply to medical school |
| **NIST Laboratory, Division, and Group:** | Materials Measurment Laboratory, Materials Science and Engineering Division, Polymers Processing Group |
| **NIST Research Advisor:** | Leanne Friedrich |
| **Title of Talk:** | How to protect cells during bioprinting |


**Abstract:**

Extrusion-based bioprinting may have tremendous implications in the field of tissue engineering. In its simplest form, this method of bioprinting utilizes cells that are distributed throughout a matrix (e.g. collagen or alginate). This ink is then passed through a nozzle and written as filaments that layer on top of one another to create more complex shapes. Optimization of material properties and printing parameters that take into account cellular needs, therefore, is a crucial step toward effective fabrication of 3D biological structures. When cells are inside the printing nozzle, they may experience damage due to high shear stresses. For example, they may rupture or lose normal function because shear stresses can disrupt signals within the cell. Previously, simulations indicated that more viscous materials, smaller nozzle sizes, and higher flow speeds correlated with cell damage. To establish guidelines for how to reduce this stress and ultimately improve cell viability and proliferation during and after bioprinting, this work experimentally examined the effects of multiple printing variables, including material identity and concentration, nozzle size and shape, as well as flow speed, on cell survival. 293T and human chondrocyte (HC) cells were mixed with gelatin/media inks of varying concentrations and were subsequently extruded through a bioprinting nozzle onto a substrate as straight lines. Their viability and proliferation were then measured using immunofluorescence staining. This experiment sheds light on how to most effectively print gelatin-based cell laden bioinks and provides useful data for those working with similar materials. Verifying previous simulation data, these measurements identify generalizable trends about how to protect cells and correct defects during the printing process. In the future, we plan to test more cell types to widen this experiment's applicability across different fields of tissue engineering and regenerative medicine.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

**Name:** Lukas Marple

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

**Major:** Biology

**Academic Standing**
**(Sept. 2023):** Senior

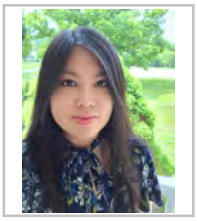
**Future Plans**
**(School/Career):** Graduate School/Medical Work (CRNA or PA)

**NIST Laboratory,**
**Division, and Group:** Material Measurement Laboratory (MML), Division 644

**NIST Research**
**Advisors:** Sandra Da Silva and Aaron Urbas

**Title of Talk:** Advancing Metabolomics: How can we Improve Fecal Metabolite Extraction?

**Abstract:**
The gut microbiome is a complex environment crucial to maintaining human health and disease prevention. The fecal material that moves through the gut is just as complex. The study of gut metabolome could aid in improving disease diagnosis and medical research. Analytical methods to extract and quantify metabolites in fecal matter have improved but finding new and efficient ways to increase the effectiveness of metabolomics analysis is critical. The main goal of this research project is to improve small molecule extraction of fecal material using ultrasonication. In our initial investigation, we sought to test different ultrasonication parameters to extract metabolites from pooled human stool. The pooled stool is from four donors and was manufactured by BioIVT as a precursor of RM8048. In the experiment, four experimental conditions were tested, varying parameters including cycle per burst intensity and ultrasonication time. Each sample was ultrasonicated and then extracted. The sample extract was analyzed by proton nuclear magnetic resonance ($^{1}$H NMR) and data was processed using MNova and Chenomix software. The result showed that ultrasonication significantly increased the extraction of metabolites compared to a control (no ultrasonication). Cycles per burst and time had the most impact. In addition, we have tested the impact of thawing conditions on the stability of the metabolites during sample processing. Samples were thawed in two conditions: room temperature and 4 $^{o}$C. They were then extracted and run by $^{1}$H NMR.
This ongoing project aims to improve and develop an approach to analyze human stool metabolome while maintaining the stability of the metabolites during the analytical workflow. The approach developed herein contribute to the NIST microbial metrology program to develop and quantify reproducible human fecal reference materials relevant to the gut metabolome community and lays the groundwork towards setting measurement standards for diagnostics and healthcare implications.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Megan Nguyen |
| **Academic Institution:** | University of Maryland, Baltimore County |
| **Major:** | Biochemistry and Molecular Biology |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | To attend graduate school and conduct biomedical research |
| **NIST Laboratory, Division, and Group:** | MML; Biosystems and Biomaterial Division; Complex Microbial Systems Group |
| **NIST Research Advisor:** | Dr. Scott Jackson; Dr. Stephanie Servetas |
| **Title of Talk:** | Investigation of the Relationship Between Diet and the Human Gut Microbiome |


**Abstract:**

The human gut microbiome (HGM) is the largest set of diverse microorganisms in the human body. In recent decades, research in this area has been of much interest due to its link to a multitude of human health conditions from digestion and metabolism of medication to chronic disease and other ailments. Due to this importance, it is crucial to understand the interdependent relationship between the HGM and features of our daily lives more specifically, our diets. In order to do this, we analyzed fecal samples and dietary logs from donors so that we can gain insights of how different food items and nutritional components influence the HGM and vice versa.

To accomplish this, we recruited cohorts of fecal donors that differed based on their diets. Each donor completed a diet log for at least a 7-day period before the fecal donation. Dietary logs from the donors were analyzed by quantifying and qualifying the macronutrients and other active ingredients. This information was contrasted between different donors and dietary preferences. In parallel, the fecal samples were analyzed by next-generation sequencing (NGS) to detect and quantify the various microbial organisms and potentially detect residual plant and animal DNA from their diets. This metagenomic DNA sequence data was then compared to NCBI's GenBank reference genome database to make connections relating different diets and the genetic signatures found in the fecal material of different donors.

From the DNA sequence data, we were able to identify plant and animal DNA signatures that correlated to the reported diets of the donors. Furthermore, we found correlations between the microbial genetic signatures and the dietary preferences of the donors. This work is building a foundation for improving HGM measurements and the development of future microbiome standards. This project supports the advancement and adoption of clinical applications that target the HGM and contributes to a deeper understanding of the human microbiome.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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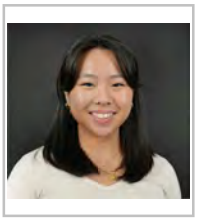
|---|---|
| **Name:** Maria Lindsey | |
| **Academic Institution:** Georgia Institute of Technology | **Major:** Biomedical Engineering |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Pursuing both a Ph.D. program in biomedical engineering and a medical degree |
| **NIST Laboratory, Division, and Group:** | MML, Biosystems and Biomaterials Division, Biomarker and Genomic Sciences Group |
| **NIST Research Advisor:** | Dr. Diane Nelson, Ph.D. |
| **Title of Talk:** | Comparison of Traditional In Vitro Viability Assays |


**Abstract:**

Extracellular vesicles (EVs) are lipid bilayer bound vesicles secreted by cells into extracellular space. EVs, as a broader categorization, include apoptotic vesicles (largest in size), microvesicles, and exosomes (smallest in size). EV sizes can range anywhere from 30 – 5,000nm, and encapsulate protein, lipids, RNA, and DNA for intercellular communication. Previous work in the field of EVs suggest their potential role in cell signaling as a warning signal for lung toxicity and airway remodeling. Lung epithelial cell viability can be used to determine the feasibility and reproducibility of secreted EVs as a long-term toxicity/airway remodeling assessment.

In this study, A549 (adenocarcinomic human alveolar basal epithelial cells) will first be exposed to toxicants including Polyethyleneimine–conjugated gold nanoparticles (Au-PEI NP) at 0.32 – 12 ug/mL and CdSO4 (0.5 – 1 mmol/L) as a positive chemical control for 24 hours. After exposure, toxicity will be evaluated by using traditional viability assays such as proliferation, LDH, MTS and the comet assay, and by observing changes in the secreted EVs size and concentration via microfluidic resistive pulse sensing. EVs secreted from lung epithelial cells will then be delivered to recipient fibroblast cells. The resulting phenotypic changes (collagen type I and α-SMA) in the recipient fibroblast cells will be measured via Western blotting. Thus far, preliminary results of the LDH assay show 5,000 cells to be the optimal number for reproducible results.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|---|
| **Name:** Jennifer Li | | | |
| **Academic Institution:** | University of Maryland College Park | **Major:** | Neuroscience, Information Science |
| **Academic Standing (Sept. 2023):** | Senior | | |
| **Future Plans (School/Career):** | MD, MD/PhD | | |
| **NIST Laboratory, Division, and Group:** | MML, Biosystems and Biomaterials Division, Biomarker and Genomic Sciences Group | | |
| **NIST Research Advisor:** | Dr. Nathanael Olson | | |
| **Title of Talk:** | Development of visualizations for the Genome In A Bottle data portal | | |

**Abstract:**

The Genome in a Bottle (GIAB) Consortium is a project led by NIST to authoritatively characterize the genome sequence of seven individuals. These seven genomes have been extensively sequenced by all commercially available sequencing technologies capable of whole human genome sequencing. While most of this data is publicly available it is not always well documented and easy to find. The Genome in a Bottle data portal is a project currently underway that will allow users to more easily find relevant datasets and explore available metadata using various data visualization techniques. This specific project involves developing the code and resulting plots in R for implementation in the GIAB data portal.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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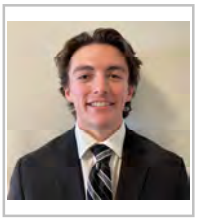
|---|---|
| **Name:** Jane Jou | |
| **Academic Institution:** University of Maryland, College Park | **Major:** Biochemistry and Art History |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Graduate School |
| **NIST Laboratory, Division, and Group:** | Material and Measurement Laboratory, Biomarker and Genomic Sciences Group |
| **NIST Research Advisor:** | Zhiyong He |
| **Title of Talk:** | Detection of EML4-ALK Fusion Cancer Biomarker in Liquid Biopsy by EFIRM |


**Abstract:**

Lung cancer is one of the leading causes of cancer-related deaths, globally. Specifically, in cases where patients present with non-small cell lung cancer (NSCLC), it is crucial to detect the cancer at an early stage, as more severe symptoms tend to stay hidden until the cancer advances. Early detection can lead to possible tumor removal, increasing the 5-year survival rate. Some NSCLC molecular mechanisms of pathogenesis are known, such as mutations of the EGFR gene, ALK fusion, etc. Mutant DNA or RNA released from tumor cells present in circulating body fluid such as plasma, saliva, urine, and can be used to detect the presence of tumor cells at early stage. Liquid biopsy (LB) samples utilize circulating tumor DNA/RNA and are minimally or non-invasive, depending on the type of sample taken (plasma/blood or saliva). Liquid biopsies can be taken before symptoms present, therefore are useful for early-stage disease detection and disease screening/progression. A newly emerged technology termed EFIRM (electric field-induced release and measurement) has shown to be highly sensitive and accurate in its detection of EGFR mutations associated with NSCLC in liquid biopsies. Previously, the Wong Lab from UCLA reported that EFIRM detected EGFR L858R and T790M mutant DNA but, not RNA from liquid biopsies. However, in theory since RNA is more abundant than DNA in LB samples and DNA-RNA binding is relatively stronger than DNA-DNA binding, we hypothesized that EFIRM can detect mutant RNA in liquid biopsies. The EML4-ALK gene fusion is one of the mutations that cause NSCLC. Since there are different genomic DNA break points that result in the same EML4-ALK gene fusion, it is easier to target mutant RNA than DNA. We tested our hypothesis and addressed whether EFIRM can detect the EML4-ALK fusion mutant DNA and RNA and what the limit of detection (minimal detectable DNA/RNA copy numbers) is. The data proved that EFIRM was able to detect both EML4-ALK fusion DNA and RNA synthetic oligonucleotides. RNA detection was relatively more sensitive than DNA detection.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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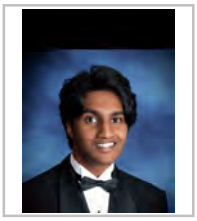
|---|---|
| **Name:** | Walter J Adamy Jr |
| **Academic Institution:** | Rochester Institute of Technology |
| **Major:** | Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | 3rd Year |
| **Future Plans (School/Career):** | Complete my Masters Degree and continue with a career in motorsports |
| **NIST Laboratory, Division, and Group:** | Material Measurement Lab, Materials Measurement Science Divission, Security Technologies Group |
| **NIST Research Advisor:** | Alexander K Landauer, Amanda L Forster |
| **Title of Talk:** | Comparison of High-Rate and Quasi-Static Mechanical Testing for Aged and Unaged Single High Strength Fibers for Use in Body Armor Applications |


**Abstract:**

In 2003 there was an unexpected in-service failure of a piece of ballistic-resistant body armor. In the wake of that incident, the scientific community has made much headway in characterizing the age- and storage-dependent properties of the constituent fibers that make up these pieces of armor, with the goal being to improve prediction of how the armor will perform. The data collected should accurately capture how the fiber will react under realistic use conditions so that accurate predictions and judgments can be made. There has been extensive research done towards characterizing these fibers at slow (quasi-static) strain rates and limited research studying the fibers at fast (dynamic) rates. Characterizing neat fibers taken directly off the manufacturer's spool only capture part of the necessary data. As in the presented example, exposure to heat and humidity effects the fibers and has led to premature in-service failures. In order to get the complete picture for the predictions it is necessary to test both unaged and aged fibers at quasi-static and dynamic strain rates. Thus, combining aging and varying of strain rates from quasi-static to dynamic is the focus of this summer's research.

Using a combination of a FAVIMAT Textile Tester and a Split-Hopkinson (Kolsky) Bar we can cover a range of displacement rates from 0.1 mm/min to roughly 1 m/s. Single fiber Kolsky bar testing is a relatively unique capability that involves significant design, calibration, and validation of the measurements taken. Using these two techniques, unaged fibers were tested at various rates within that range and the force-displacement and ultimate stress and strain were recorded. Then, a spool of fiber that was aged 1 year at 70°C and 75% relative humidity was used for the same tests. Using this information we can inform guidelines for the service life of body armor, preventing any more failures like the one in 2003 and continue to enable confident use of armor by law enforcement and military users.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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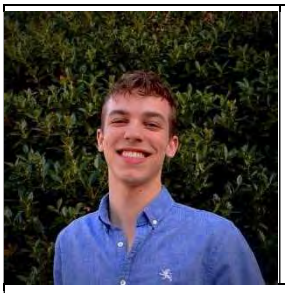
|---|---|
| **Name:** Ryan Punith | |
| **Academic Institution:** University of Maryland, College Park | **Major:** Materials Science & Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Enter materials engineering industry for a few years in metallurgy or mechanical testing, and then get Master's degree for research in fusion reactors. |
| **NIST Laboratory, Division, and Group:** | 643.10 |
| **NIST Research Advisor:** | Dr. Alexander Landauer |
| **Title of Talk:** | Mechanical Testing of Heterogenous, Graded Impact Protection Materials |


**Abstract:**

Protective equipment such as football helmets often uses layered materials, e.g., polymer foams of varying stiffness, to provide comfort and impact protection. To better design this equipment, the mechanical performance of the impact mitigation material layer, and the interaction between the layers, must be understood. This is often accomplished by measuring the deformation of the material in response to a known applied force. An effective technique to measure deformations in heterogenous materials, such as layered foam, is digital image correlation (DIC). DIC uses camera optics in tandem with image-tracking software to measure the displacement over time across points on a material's surface as specimens undergo deformation. This work focuses on mechanical characterization of conventionally layered and novel functionally graded foam materials using digital image correlation techniques.

The conventionally layered foams were constructed as stacked layers of vinyl nitrile, polyethylene, and neoprene foams. Some specimens were also modified in the e-beam with custom masks to impose a functional gradient. To calibrate the dose sensitivity of the vinyl nitrile foam, the fresh foams were subjected to e-beam dosages ranging from 0.1 kGy to 100 kGy and these were tested for changes in stiffness. Mechanical testing was conducted with a universal testing machine and a custom instrumented drop tower, and 2D-DIC analysis was conducted with open-source MATLAB scripts. To obtain a more thorough view of the specimens' mechanical response, stress-strain data was observed for macroscopic changes in strength and DIC strain fields were used to investigate changes in strain distribution due to layering and functional gradation. Transmitted force and peak impactor accelerations from the instrumented drop test are used to compared layering efficacy.



# SURF Student Colloquium

NIST – Gaithersburg, MD August 1-3, 2023

**Name:** Bradlee Rich

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|---|---|---|
| **Academic Institution:** | Eastern Kentucky University | **Major:** Forensic Chemistry |
| **Academic Standing (Sept. 2023):** | Senior | |
| **Future Plans (School/Career):** | Obtain a forensic position at the state or federal level | |
| **NIST Laboratory, Division, and Group:** | MML, 643, 10 | |
| **NIST Research Advisor:** | Amanda Forster | |
| **Title of Talk:** | Solving the worlds textile waste problem one blend at a time | |

**Abstract:** Fast fashion has put the world's textile waste production into overdrive. A 2018 study by the EPA showed that textiles are the fastest growing waste stream in municipal solid waste audits in the U.S. Additionally, only a mere 15% of textiles are ever recycled nationwide and thus, an increasing need to develop better recycling methods for clothing made from synthetic polyesters, such as polyethylene terephthalate (PET), has arisen. To facilitate reclamation of this waste stream, rapid, accurate sorting is required. Near-infrared (NIR) spectroscopy has been demonstrated for use in sorting of other waste streams, such as single-use plastic, and shows promise to enable rapid sorting of textiles. Through the use of laboratory analytical techniques such as Fourier transform – near infrared spectroscopy (FT-NIR), thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC), characterization of virgin PET, recycled PET (rPET), cotton, and blends of each is performed. Results of this analysis serve to create a systematic study of blend percentages, creating a data series that relates material blends to its physical properties and develops a better understanding of recycling routes for polyester fibers. This information can then be exchanged with corporations to enable or influence new and existing circular economy efforts.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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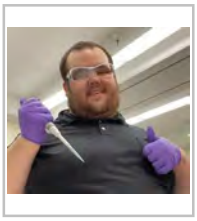
|---|---|
| **Name:** | Maxwell Mevorah |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Chemistry |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Pursue PhD in Green Chemistry |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory |
| **NIST Research Advisor:** | Charlotte Wentz & Amanda Forster |
| **Title of Talk:** | Synthesis and Characterization of Metal-Impregnated Lewatit for Direct Air Capture (DAC) |


**Abstract:**

Due to its significant presence in our atmosphere, carbon dioxide (CO2) plays an ever-important role in the growing climate crisis. Like glass on a greenhouse, CO2 and other "greenhouse gases" trap thermal energy from the Sun, raising the temperature below. To stave off a runaway greenhouse effect, we must not only transition away from fossil fuel dependence but also actively remove CO2 from the atmosphere — a technology termed Direct Air Capture (DAC).

Though there are various ways to employ DAC, the safest and most well understood method relies on large fans and the principle of adsorption, where a solid holds another solid, liquid, or gas on its external or internal surface(s). The fans blow vast quantities of air onto a material that adsorbs the very dilute CO2 present in the air (~420 ppm) after which it can be collected and sequestered or repurposed.

In this study, Lewatit® VP OC 1065 — a weakly basic, anion exchange resin — was impregnated with copper and iron to create CO2 adsorbent materials that were then characterized based on their CO2 capacities. After soaking the resin overnight and rinsing with deionized water (DI), the sample was soaked in a flask of either CuCl2 or FeCl2. Once saturated, the sample was rinsed with DI, activated, by rinsing with salt solution and DI or heating to 100˚C, and analyzed via thermogravimetric analysis (TGA), a humidity-controlled gas analyzer, and microscopy. Though the data is still largely inconclusive due to a lack of sufficient repetition, the preliminary results indicate that cuprated-Lewatit samples have a greater CO2 capacity than ferrous-Lewatit samples, which have a greater capacity than pure Lewatit. While none of the samples tested appear to have capacities sufficient for their intended purpose, this may turn out to be incorrect following additional testing.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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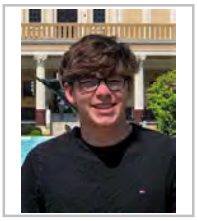
| **Name:** Tyler Hicks | | | |
| **Academic Institution:** | Swarthmore College | **Major:** | Chemistry |
| **Academic Standing (Sept. 2023):** | Senior | | |
| **Future Plans (School/Career):** | PhD in Chemistry; Professor in Chemistry | | |
| **NIST Laboratory, Division, and Group:** | MML Division 642; Polymers and Complex Fluids Group | | |
| **NIST Research Advisor:** | Dr. Christopher Sims | | |
| **Title of Talk:** | Exploration of Parameters for Carbon Nanotube Separations via Automated Fluorescence Titration | | |

**Abstract:**

Single-wall carbon nanotubes (SWCNTs) have a variety of useful optical, electronic, thermal, and mechanical qualities that would be ideally harnessed for various applications, including biotherapeutics, sensors, and energy storage. However, synthetic methods do not produce single SWCNT species but rather mixtures of various species which limit their utility for some of their potential uses. Therefore, the efficient and reproducible separation and refinement of specific species is an intensely sought after objective. One such separation system is aqueous two-polymer phase extraction (ATPE) which utilizes the difference in solvation energies in each of the two polymer phases to distribute a specific SWCNT species into a specific polymer phase. Interestingly, one can track these phase transitions using fluorescence spectroscopy. Previous NIST research has shown that the presence of various third components can shift these extractions to much favorable conditions. Utilizing a novel automated fluorescence titration technique, the exploration of this massive phase space becomes vastly more attainable. This project focuses on the addition of various salts and third surfactants to attempt to shift ATPE to more industrially favorable conditions.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Colin McCarragher

**Academic Institution:** Tufts University | **Major:** Biochemistry

**Academic Standing (Sept. 2023):** Senior

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

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

**NIST Research Advisor:** Phillip Pickett


**Title of Talk:** Analysis of Polyzwitterion Solutions Using Dynamic Light Scattering


**Abstract:**

Polyzwitterions are a class of polyelectrolytes that contain both a positive and negative charge on each monomer repeat unit. The close proximity of these charges creates ion-dipoles that interact and drive the stimuli-responsive behavior of polyzwitterions. Unlike other polymers, polyzwitterions are subjected to the anti-polyelectrolyte effect that describes the dissociation of inter- and intra-polymer interactions in the presence of salt. Polyzwitterions also exhibit upper critical solution temperature (UCST) behavior, in which the polymer phase separates from solution below a critical temperature in water. These unique properties are the basis for using polyzwitterions for a variety of applications, ranging from water treatment to use as drug delivery vehicles. However, despite their distinctive properties, the chain dynamics of these macromolecules are not well understood, particularly near their phase boundaries. To understand the polyzwitterion phase behavior further, we synthesized and characterized a model polyzwitterion, pAPAPS, with a variety of molar masses. The temperature-concentration phase diagrams were determined for each molar mass via cloud point measurements. Additionally, the polymer dynamics were probed using dynamic light scattering (DLS) as the solutions approach their phase boundaries from one phase. This work provides insight into how molar mass and temperature affect the inter-polymer ion-dipole interactions as reflected by the concentration-dependent diffusion coefficients. Understanding these phenomena at the early stages of phase separation will aid in the development of predictive structure-property models, which will increase our ability to precisely tune the self-assembly of polyzwitterionic-based materials with UCST behavior for environmental and biomedical applications.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Gabrielle Schumacher | |
| **Academic Institution:** University of Maryland | **Major:** Aerospace Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate School |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory (MML) |
| **NIST Research Advisor:** | Marcos A. Reyes-Martinez and Ami Ahure Powell |
| **Title of Talk:** | Liquid Crystal Elastomer Membranes for Enhanced Impact Resistance of 3D Structures |


**Abstract:**

Biological materials such as the cuticle of the armored beetle, the club of the mantis shrimp, and the puncture-resistant fishscales of the Arapaima, all share a characteristic hierarchical helical (chiral) packing of structures across length scales. This structure allows them to be extremely tough and withstand repeated impact without catastrophic fracture propagation. In this study, we explore how chiral order can enhance the impact resistance of soft materials. Specifically, we focus on liquid crystal elastomers (LCE) and how chiral order influences the impact resistance of three-dimensional (3D) skeletal structures. We hypothesize that the structure of chiral liquid crystal elastomers (CLCE) increases impact strength, while also resisting compression and penetration. Four 3D skeletal structures with different mean curvatures are coated with amorphous LCE and compared to CLCE membranes to unravel the influence of chiral order on impact resistance. Drop mass experiments, combined with high-speed videography, are performed using a 28g mass and are able to reach a range of energies from 10-2 J to 10-1 J, corresponding to impact speeds of between 1 m/s - 5 m/s. The results are then used to measure the peak transmitted force, fracture resistance, and fatigue behavior across all materials and geometries. We complement impact tests with Digital Image Correlation (DIC) to accurately quantify the global and local strains resulting from impact events and characterize how strain localization is affected by the different LCE membrane. Our results show that CLCE coating improves the strength and resilience of 3D skeletal structures under impact, compared to structures with amorphous LCE coating and without coating. This is surprising given that the chiral nematic order in our LCEs is an interfacial phenomenon that extends only 10um into the thickness of the membrane (nominally over 100um thick). This form of thin layer enhancement has the potential to be used in many applications, from improving the design of materials for impact mitigation, to the aerospace industry where it could be used to enhance the skin of an airplane fuselage.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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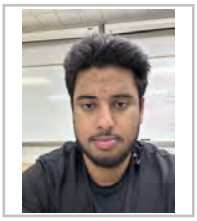
|---|---|
| **Name:** Mia Merritt | |
| **Academic Institution:** Morgan State University | **Major:** Engineering Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Earn a PHD in physics |
| **NIST Laboratory, Division, and Group:** | MML, Division 242, Group 03 |
| **NIST Research Advisor:** | Dr.Frank Abel |
| **Title of Talk:** | Study of Iron Oxide Nanoparticle Dynamics Based on Surface Functionalization for Magnetic Particle Imaging |

**Abstract:**

Magnetic Particle Imaging (MPI) is a technique that utilizes the nonlinear response of magnetic nano-objects (MNOs) to produce an image. Recent findings have shown that chain formation of high crystal quality iron oxides with an oleic acid shell can yield significant improvements in signal to noise and spatial resolution [1,2], which may be related to the development of a colloidal shape anisotropy above specific drive field amplitudes [3]. The details of the chain formation are controlled by the magnetization of each MNO as well as the length of the surface functionalizing molecule. However, to be useful in biomedical imaging, the MNOs need to maintain their stabilization and properties in an aqueous environment, but the surfactant change may negatively impact this. Two approaches were considered to identify the impact of surface functionalization on 20 nm diameter iron oxide MNOs: The first method attempts to exchange oleic acid (short ligand) for carboxylic acid terminated polystyrene (long ligand), which are both soluble in toluene. The second approach uses a micelle (Tween-20) to encapsulate the particles to make them soluble in water. For these studies, the MNOs were characterized by X-ray diffraction, Raman spectroscopy, and electron microscopy. The time domain magnetic particle spectroscopy (MPS) was used to study the dynamic magnetization response of the samples and dynamic light scattering (DLS) was used to estimate the size of the MNOs in a colloidal environment. As seen previously, there is a sharp MPS response in the oleic acid functionalized particles which exhibit large aggregated (744 nm) structures in DLS. In the case of the polystyrene and micelle functionalized MNOs, the MPS response is reduced to nearly identical time domain responses. In both cases, DLS shows smaller aggregated structures, which could be a mixture of singular isolated particles, or several particles fixed within a larger molecular structure. These results suggest that the length of the surface functionalizing ligand greatly impacts chain formation and the MPS response.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|
| **Name:** Mohhamed Rafi | | |
| **Academic Institution:** University of Maryland College Park | | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Senior | |
| **Future Plans (School/Career):** | Graduate School | |
| **NIST Laboratory, Division, and Group:** | MML,Division 642, Thermodynamics and Kinetics | |
| **NIST Research Advisor:** | Daniel Wheeler | |
| **Title of Talk:** | Developing a spectral accurate solution to assess results for the Cahn-Hilliard benchmark | |


**Abstract:**

The phase field benchmark project [1] uses standardized benchmarks to provide quality assurance for phase field codes. The main function of the project is to provide adequate accuracy and uncertainty quantification for submitted benchmark results allowing helpful comparisons between different codes and control parameters. This quality assurance requires a trusted "gold standard" solution for each benchmark for comparison. This work aims to provide a "gold standard" solution as well as better error metrics for the first benchmark problem (the Cahn-Hilliard benchmark). We employ a spectral accurate solution to the Cahn-Hilliard benchmark problem as the "gold standard" solution, which is known to have a high degree of spatial accuracy. To compare different configurations, we look at a variety of error metrics including the L2 norm, 2-point spatial statistics and spectral density function. These error metrics require careful interpolation routines that preserve the original spectral accuracy of the solutions when comparing between different grid densities. Quantitative comparisons between the "gold standard" solution and results using other software frameworks, such as FiPy, can be made using these error metrics. These comparisons will be implemented on the phase field benchmark website (PFHub) to improve the automated quality assurance tools available on PFHub.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


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|---|---|
| **Name:** | Spencer Mattes |
| **Academic Institution:** | Binghamton University, State University of New |
| **Major:** | Mathematical Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | I intend to attend graduate school starting in the fall of 2024. |
| **NIST Laboratory, Division, and Group:** | Materials Measurement Laboratory, Division 642, Group 3 |
| **NIST Research Advisor:** | Dr. Kathleen Schwarz and Dr. Michael Woodcox |


**Title of Talk:** Temperature and pressure dependence of dielectric spectra based on molecular dynamics simulations


**Abstract:**

Dielectric spectroscopy provides insight into the physical and chemical properties of fluids by probing the system with electric signals across a broad range of frequencies, and measuring the resulting polarization. Compared to alternative measurement techniques that only identify direct interactions between ions (Raman, NMR, etc.), dielectric spectroscopy can be used to reliably detect intermolecular interactions across larger length scales. Consequently, there has been tremendous interest in applying dielectric spectroscopy to facilitate more efficient chemical separations in the pharmaceutical industry. Computational research has been focused on utilizing molecular dynamics simulations to identify the molecular phenomena that underlie the peaks in the dielectric spectra. Determining the origins of these peaks is paramount to improving the interpretations of experimental data, and advancing the capabilities of dielectric spectroscopy.

The fluctuation–dissipation theorem is currently the default method for calculating the dielectric spectra via molecular dynamics, since the dielectric response over a broad range of frequencies can be computed from a single simulation. However, the high computational cost required to produce reliable results at lower frequencies remains a concern. By applying alternating current electric fields resembling those used in experiment, we simulate the dielectric response of fluids at targeted frequencies to explore features within the dielectric spectra more efficiently. Furthermore, the use of classical molecular dynamics enables the exploration of the molecular and chemical phenomenon that dictate the dielectric response. In this work, the dielectric spectra are computed for multiple solvents as a function of temperature and pressure in order to establish a baseline for comparisons with the spectra of more complex solutions.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|
| **Name:** Nishwanth Gudibandla | | |
| **Academic Institution:** | University of Maryland, Baltimore County | **Major:** Physics & Computer Science |
| **Academic Standing (Sept. 2023):** | Junior | |
| **Future Plans (School/Career):** | Attend Graduate School for a Doctorate in Physics | |
| **NIST Laboratory, Division, and Group:** | Materials Measurement Lab, Material Science & Engineering Division, Thermodynamics & Kinetics Group | |
| **NIST Research Advisor:** | Daniel Wines | |
| **Title of Talk:** | Understanding the Magnetic Properties of 2D Vanadium Diselenide with Density Functional Theory | |


**Abstract:**

Monolayer transition metal dichalcogenides (TMDs) are an emergent category of two-dimensional (2D) materials that excel in a wide variety of electronic and technological applications. 2D magnetic materials are also of great interest due to their potential spintronic applications. VSe2 is a TMD that exhibits strong magnetic properties, with multiple studies controversially claiming that it is ferromagnetic at room temperature. In addition, competing magnetic and non-magnetic states are predicted to exist in VSe2, which can drive the formation of charge density waves (CDW). Furthermore, the material exists in two phases (H and T-phase) that each correspond to a unique set of properties. Taking a computational approach, we use Density Functional Theory (DFT) to predict the electronic and magnetic properties of T-phase VSe2. With varying degrees of accuracy and complexity, we aim to identify the stability of various magnetic orientations in T-VSe2 and benchmark the results with experiments. In addition, we study the response of the material to external factors such as strain, vacancies, and impurities. These calculations will serve as high-quality reference data that can be utilized by experimentalists who wish to characterize T-VSe2 for industrial applications.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Aubrey Augustine

**Academic Institution:** Tulane University | **Major:** Physics and Russian

**Academic Standing (Sept. 2023):** Junior

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

**NIST Laboratory, Division, and Group:** MML, Materials Science and Engineering Division, Polymers Processing Group

**NIST Research Advisor:** Anthony Kotula


**Title of Talk:** Assessing Magnetic Levitation for Plastics Densimetry


**Abstract:**

Existing density measurement techniques can only measure a single sample at a time, which makes the process time-consuming for measuring the properties of multiple plastics or assessing bath-to-batch variation. However, using technology as simple and inexpensive as magnets to produce magnetic levitation (MagLev), density measurements can become quicker and more cost-effective. In MagLev, gravity, buoyancy, and magnetic forces act on a sample placed in the magnetic field generated between two magnets positioned with like-poles facing each other. This force balance results in samples equilibrating at a height between the magnets that is proportional to density. Multiple samples can be equilibrated simultaneously to improve measurement throughput, but MagLev requires samples that are diamagnetic, and the presence of paramagnetic impurities in samples will affect density measurement accuracy. Although pure plastics are diamagnetic, the pigments and additives that make plastics appealing to consumers are often paramagnetic (and have different densities than the pure plastic), which could be a source of measurement error for this technique.

To test the accuracy of MagLev-based density measurements, we used polylactic acid (PLA) with a variety of pigments and densities. Density is a function of the sample crystallinity, which is varied by annealing the samples for different durations at intermediate temperatures between the glass transition and melting. Polarized optical microscopy measurements during isothermal crystallization are used to determine suitable annealing conditions. Four different sample colors - white, black, red, and “natural”, which contains no colorants - are used to assess sensitivity to pigment properties. The equilibrium height, magnetic field strength, and individual susceptibilities of the paramagnetic and diamagnetic materials are then used to determine the effect of pigments on overall magnetic susceptibility, a critical property in the MagLev force balance. The effect of these property differences on density accuracy is directly tested by comparing MagLev-based density measurements with those from a laboratory balance. These results demonstrate the robustness of MagLev to characterize common pigments in commercial plastics, which is useful in developing this technique for applications in sample purification and plastics separation for recycling.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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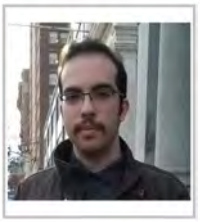
| **Name:** Leila Clark | |
| **Academic Institution:** Pace University | **Major:** Biology |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | To get my PhD in neuroscience. |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory (MML), Division 642, Group 6 |
| **NIST Research Advisor:** | Benjamin Dolata |
| **Title of Talk:** | Investigating Shear-Induced Disentanglement Using the Slip-Link Model |

**Abstract:**

In polymer extrusion 3D printing a polymer is melted by a heated printer head and deposited layer by layer to form a three-dimensional object. The polymer melts used in these processes are dense, meaning nearby chains constrain each other's motions; these constraints are called entanglements. These entanglements enhance the polymer's resistance to deformation, resulting in improved tensile strength, toughness, and dimensional stability of printed parts. Disentanglement occurs when polymers are under flow, which simulations have suggested can lead to weakened welds between printed layers. Experimental verification of this proposed mechanism requires a method to measure how entanglements change under flow. Recent experiements have suggested that the dependence of pressure-controlled capillary rheology on molecular weight can be used to measure disentanglement under flow. We have simulated sliplink chains (a coarse-grained mean-field model of entangled polymer melts) to investigate the feasibility of using pressure-controlled rheology to study disentanglement. We use the Green-Kubo relation to find the dependance of the zero-shear viscosity on molecular weight and find that the spliplink model reproduces tube statistics. The sliplink chains disentangle at heigh stresses, leading to Rouse scaling of the viscosity due to diffusion of the dangling ends of the chain. These results confirm that pressure-controlled rheology can be used to measure shear-induced rheology and highlight the importance of including dangling end dynamics in sliplink simulations.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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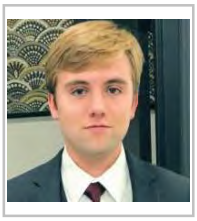
|---|---|
| **Name:** Leonardo Borchert | |
| **Academic Institution:** The George Washington University | **Major:** Aerospace Engineering |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Get a PHD in Aerospace Engineering & design advanced particle and plasma propulsion systems for air and spacecrafts. |
| **NIST Laboratory, Division, and Group:** | Materials Measurement Lab., Materials Measurement Science Div., Nanomechanical Properties Group |
| **NIST Research Advisor:** | William Alexander Osborn & Lakshmi Ravi Narayan |
| **Title of Talk:** | Optimization of Nano-Calorimetry Sensors using Finite Element Simulations |

**Abstract:**

The ability to measure and analyze a material's thermal properties and characteristics plays an important role in material science. Measuring the effects however of rapid temperature changes on materials has always been an issue with classic calorimetry methods. Nano-calorimetry uses chip sensors in lieu of crucibles in furnaces to perform thermal analysis on nano-scale materials, often at very high heating and cooling rates. To simulate several different capabilities of different sensors, SolidWorks, a 3D modeling software was used to design these sensors. Once created, the designs were imported into ABAQUS, a finite element simulation software. Finite element simulations were used to determine the resonant frequency of the nano-calorimetry sensors, which will allow for the mass of a sample to be calculated based on the change in its resonance frequency. Finite element simulations of the coupled thermal-electric type were also run to determine the temperature distribution in the sensor during heating experiments. Having a more even spread of heat throughout the sample correlates to more accurate results. Analyzing the data collected from the simulations, it was discovered that the slight adjustment of the mesh sizes for the finite elements caused drastic data variations along each mode. Running several simulations with different mesh sizes was done to identify a possible trend within the error rate of finite element meshing. These simulations were also performed on candidate designs for the redesign of the nano-calorimeter sensor, and the optimum was selected based on these results.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Connor Davison | |
| **Academic Institution:** Lehigh University | **Major:** Materials Science and Engineering |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Graduate from Lehigh with a B.S. in materials engineering and a minor in nanotechnology |
| **NIST Laboratory, Division, and Group:** | MML, 643.08 |
| **NIST Research Advisor:** | Russell Maier |
| **Title of Talk:** | Improving Toughness of Ceria-Based Oxygen Ion Conductors |


**Abstract:**

Electroceramic materials are used in a wide variety of applications that include piezoelectrics (ultrasonic transducers, energy harvesters), ferroelectrics (ferroelectric random access memory, electrocalorics), dielectrics (multi-layer ceramic capacitors, memristors) to name a few. The perovskite structure is a complex oxide and its functionality can be designed for specific applications by tuning the magnetic, electronic, or mechanical properties by carefully engineering the chemistry, defect properties, and microstructure of the material. Because they are oxides, the stoichiometry, defect chemistry, and polycrystalline microstructure is heavily influenced by the oxygen atmosphere during processing.

This presentation will focus on the redox-active perovskite CeAlO3. The goal of this project is to synthesize a material that will have the oxygen ion conducting capabilities of CeO2 with enhanced toughness due to the presence of nano-sized grains of Al2O3 in the microstructure. We use non-conventional processing techniques, like spark plasma sintering (SPS), and highly reducing environments to control the stoichiometry and microstructure of this material. SPS is a sintering process that operates much faster than conventional sintering while also applying pressure to the sample. We reoxidize the SPS sintered and reduced samples of CeAlO3 which causes the cerium aluminate to decompose into nano-sized grains of ceria and alumina. Microscopy is used to observe the resulting microstructure to confirm the presence, phase, and size of these grains. Once samples can be synthesized with adequate microstructure, larger samples are synthesized and machined into bars for four-point bend testing to determine the mechanical properties of the ceramic. This research will provide novel insights into methods to improve the mechanical properties of ceramics using redox-driven processes.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


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|---|---|
| **Name:** | Alison Hecht |
| **Academic Institution:** | Louisiana State University |
| **Major:** | Biochemistry |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | PhD |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory (MML), Materials Science and Engineering Division (MSED), Polymers Processing Group (Group 6) |
| **NIST Research Advisor:** | Julia G. Murphy |


**Title of Talk:** Exploration of diblock copolymer blend thin films to understand multicomponent system morphologies


**Abstract:**

Block copolymers are attractive candidates for next-generation nanotemplating applications due in part to their self-assembly into periodic nanostructures. Blending two different block copolymers creates a multicomponent system that can be readily tuned to access morphologies and domain spacings different from those in the individual copolymers. An exploration of thin films prepared from diblock copolymer blend solutions was conducted to understand the morphologies that form from these multicomponent systems and how they compare to those of single diblock copolymer films. Thin films were prepared from blends of poly(styrene-block-4-hydroxy styrene) (PS-b-P4OH) and poly (2-vinylpyridine-block-methyl methacrylate) (P2VP-b-PMMA), over a range of molecular weights and blend ratios. Film thicknesses were then measured with ellipsometry, and the surface structure was characterized with atomic force microscopy (AFM) topography and phase imaging. The resulting morphologies and domain compositions were determined through AFM image analysis of the domain sizes and by comparison to X-ray scattering measurements on bulk samples. The thin films will be further characterized with resonant soft X-ray scattering (RSoXS).

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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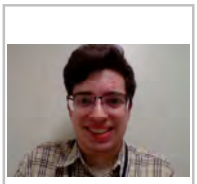
| **Name:** Evan Freeland | | | |
| **Academic Institution:** | The Ohio State University | **Major:** | Materials Science & Engineering |
| **Academic Standing (Sept. 2023):** | Senior | | |
| **Future Plans (School/Career):** | Graduate School | | |
| **NIST Laboratory, Division, and Group:** | MML, MATERIALS MEASUREMENT SCIENCE DIVISION, MICROSCOPY AND MICROANALYSIS RESEARCH GROUP | | |
| **NIST Research Advisor:** | Donald Windover | | |
| **Title of Talk:** | Thickness Measurement of Gallium Phosphide Films on Silicon with Micro-X-Ray Fluorescence | | |


**Abstract:**

Thin films, with thicknesses ranging from less than a nanometer to hundreds of nanometers, are an integral part of any modern electronic device. A fast and repeatable measurement technique is needed for measurement of film thickness, both post-processing and in-situ during film growth. X-ray fluorescence (XRF) is a promising technique for this role. XRF works by measuring the intensity of elemental characteristic x-ray energies emitted when an electron relaxes to a lower energy state in an atom. By measuring fluorescence intensity for films of varying thicknesses and plotting the results against thickness measurements from an SI-traceable method, a calibration curve can be constructed and used to assess the thickness of unknown films. Reliable application of this technique requires understanding of non-idealities in the sample and the process. Non-uniformity in film thickness must be accounted for when interpreting measurements. An appropriate fitting procedure must be created for reliable measurement of x-ray line intensities, which accounts for background bremsstrahlung, pile-up, Compton scattering, and diffraction. In this study, a series of GaP films on Si substrates, grown with MOCVD, were characterized with XRF. GaP-Si films are of great interest for LEDs, high-efficiency III-V solar cells and other opto-electronic devices due to the low lattice mismatch between GaP and Si. XRF maps were taken to study thickness non-uniformity, and high-precision measurements were taken with X-ray reflectivity (XRR). Spectra were quantified with both commercial and open-source software. Between 40nm and 290 nm for our films, the Ga line intensity is directly proportional to the thickness measured by XRR.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Arden Dombalagian |
| **Academic Institution:** | Georgetown University |
| **Major:** | Physics |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Graduate School, PhD in Physics, Research |
| **NIST Laboratory, Division, and Group:** | Materials Measurement Laboratory, Materials Measurement Science Division, Nanomechanical Properties Group |
| **NIST Research Advisor:** | Dr. Feng Yi |
| **Title of Talk:** | Nanocalorimetry for Carbon Capture Materials Characterization |

**Abstract:**

I have been working on nanocalorimetry, which is a chip-based thermal analysis technique capable of measuring phase transformations, adsorption and chemical reactions at very high heating and cooling rates. A nanocalorimeter sensor consists of a suspended silicon nitride membrane (100 nm) to reduce the thermal mass and a platinum thin film functioned as the heater and temperature sensor. I will calibrate over 100 nanocalorimeters. Based on the calibration data, I will analysis the data using Python and test/validate a new temperature calibration strategy based on recorded power during resistive heating instead of using a sophisticated optical method to measure the temperature. Then the calibrated nanocalorimeters will be used to characterize the carbon capture materials by measuring the adsorption/desorption process. Additionally, I have been helping optimize the nanocalorimetry measurement circuit to improve the measurement sensitivity.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Ryan Kim | |
| **Academic Institution:** University of Maryland: College Park | **Major:** Materials Science Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate school or industry with high social/environmental impact |
| **NIST Laboratory, Division, and Group:** | MML |
| **NIST Research Advisor:** | Aaron Gilad Kusne |
| **Title of Talk:** | AELF multiagent machine learning to map transfer data |

**Abstract:**

In Situ characterization tools are often not as descriptive as Ex Situ characterization tools. This means that calibration of In Situ tools as a function of Ex Situ data is important especially when trying to translate research done in first principles to a marketable product. One issue is that Ex Situ data is often of lower dimension than In Situ results. Machine Learning and Baysiean optimization shows promise as a way to link In Situ characterization to Ex Situ results. This paper proposes use of an autonomus experiment and learning framework (AELF) device designed to educate students about this issue and provide them with tools in machine learning to solve these problems. Furthermore, we seek to demonstrate asynchronous learning in that the two experiments need not be carried out at the same time or by the same machine.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Dennis Zhao | |
| **Academic Institution:** University of Maryland College Park | **Major:** Materials Science and Engineering |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Graduate School/Researcher |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group |
| **NIST Research Advisor:** | Dr. Aaron Gilad Kusne |
| **Title of Talk:** | Analyzing Phase Diagrams Using Machine Learning |


**Abstract:**

Autonomous physical science is the future of materials science. In autonomous systems, machine learning controls experiment design, execution, and analysis in a closed loop, speeding up the process of finding new useful materials. Autonomous systems use active learning, the machine learning field of experiment design, to select subsequent experiments that maximize knowledge gained. As active learning strategies evolve, there is a growing need for reference datasets to benchmark strategies. We present three reference datasets. The datasets describe three ternary systems and contain both phase composition and simulated X-ray diffraction for different material compositions. The datasets are then demonstrated for benchmarking active learning strategies. The active learning strategies of random selection, entropy minimization, and risk minimization are benchmarked for their ability to maximize knowledge of the composition-structure relationship, i.e., the 'phase diagram'.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Tristan Charles |
| **Academic Institution:** | Haverford College |
| **Major:** | Biology and Public Health |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | I will pursure a masters degree in Public Health and Healthcare Management/Administration. |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory/Material Measurement Science Division (643)/ Group 4 |
| **NIST Research Advisor:** | Austin McDannald, PhD |
| **Title of Talk:** | Utilizing Machine Learning to Analyze Carbon Dioxide Capture Efficiency |


**Abstract:**

The Earth's temperature is increasing rapidly, the sea levels are rising, and there are major threats posed to biodiversity across the world, and much of this can be attributed to increased greenhouse gas concentrations in the atmosphere. A plausible solution to aid in decreasing the CO2 concentration in the atmosphere is Metal Organic Frameworks (MOFs). MOFs are utilized for their wide range of potential applications, such as gas absorptions, gas storage, and gas separation. The gas storage function of MOFs will be highlighted in this project. Our focus is using graph neural networks to predict materials that possess the optimal balance of capture efficiency of CO2 and purity of CO2 captured. However, our fundamental understanding of the properties of MOF materials still needs to be improved. MOF materials are envisioned to play a pivotal role in modern society and future progressions in the scientific field but the underlying crystallographic information for these materials is very ambiguous and presents a roadblock for furthering scientific research.

The aim is to train a model that can successfully predict the capture efficiency of a MOF using machine learning.In particular the use of Graph Neural Networks (GNN) to conduct high throughput screening of these hypothetical structures.Provided with accurate findings there can be conclusions drawn surrounding comparisons between different MOFs that have similar capture efficiencies as well as analysis into the specific materials present in the working models.The objective of our work is to identify materials with the capability to accelerate the decrease in the total ppm of CO2 located within the atmosphere.

# SURF Student Colloquium

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August 1-3, 2023

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| **Name:** John Paul Marquardt | |
| **Academic Institution:** University of Maryland | **Major:** Chemistry |
| **Academic Standing (Sept. 2022):** | First Year Graduate Student at NYU |
| **Future Plans (School/Career):** | Graduate School at NYU |
| **NIST Laboratory, Division, and Group:** | MML |
| **NIST Research Advisor:** | Brian DeCost |
| **Title of Talk:** | Similarity Metrics applied to Neural Networks: Examining how Material Properties are Learned |

**Abstract:**

Neural networks are a powerful tool for many applications including image recognition, generating realistic conversations, and property prediction in materials science. Neural networks are often criticized due to their inscrutability or 'black box' nature. We undertook examination of the intermediate weights of the models using similarity metrics to elucidate how neural networks learn representations of multiple material properties. Similarity metrics are useful tools for examining how closely related data points are. We examined two similarity metrics, cosine similarity and centered kernel alignment (CKA). Cosine similarity is the cosine of the angle between two points in the neural network's internal representation. The CKA of two representations of some data is the cosine distance between the dot product similarities of all data points for each representation. We compared the ALIGNN graph neural network model to similar models for structure prediction including CGCNN and EquiformerV2. We hope to show that similar material properties are learned in similar ways and to glean useful insights into how neural networks represent data.

# SURF Student Colloquium

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August 1-3, 2023

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|---|---|
| **Name:** | Andrew Celi |
| **Academic Institution:** | Rensselaer Polytechnic Institute |
| **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Graduated |
| **Future Plans (School/Career):** | A degree in chemistry |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory |
| **NIST Research Advisor:** | Talapady N. Bhat |
| **Title of Talk:** | Integrated NIST Knowledge Website |


**Abstract:**

Searching for information online requires precise wording and deciding which articles are the most relevant. The goal of the Integrated NIST Knowledge (INK) website is to simplify the process of finding information and related data. The website retrieves information from multiple databases to generate a visually appealing display of related articles. The user can choose to display the information in a force directed graph, a tree graph, a file graph, or an incremental tree graph.

Originally, the graphs were not intuitive to the user. Some nodes in the graph would show the article ID number instead of the title, thus not readily presenting information. The code is also more generalized so that in the future, other datasets may be used to create the various graphs.

Additionally, the layout of the INK website is cluttered and can cause the user to be confused. We want to clearly separate the functions of the website. Instead of swarming the user with information about people, data, publications, and patents in every search, we allow the user to specify the exact kind of data they are looking for. The website can be used by all of NIST to help find information in specific fields.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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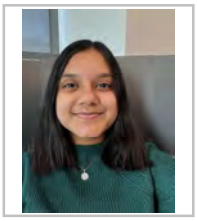
|---|---|
| **Name:** Jay Kannan | |
| **Academic Institution:** Drexel University | **Major:** Biomedical Engineering |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Currently in Drexel BS/MD program where I have a provisional admission into Drexel College of Medicine in 2026 |
| **NIST Laboratory, Division, and Group:** | MML Laboratory, Biosystems and Biomaterials Division, Cell Systems Science Group |
| **NIST Research Advisor:** | John Elliot |
| **Title of Talk:** | Using the WIPP System for Imaging Cell-Virus Interactions |


**Abstract:**

With the use of cell and gene therapies involving viral vectors becoming more prominent in clinical settings, efficient and useful analytical tools are necessary. Viruses can be characterized during a manufacturing process, and an important aspect is the functional titer level of the virus (as opposed to the physical titer) which shows the amount of virus able to infect a cell. To determine the functional titer of a virus, a viral plaque assay is used to quantify the amount of virus required to kill cells which creates a plaque. This assay is typically used as an endpoint assay; however, we can utilize live cell imaging to capture the dynamics of plaque formation allowing researchers to investigate and develop better analytical tools using this assay. An excellent method for studying viral plaque formation is to utilize high speed wide field of view timelapse imaging, although doing this creates large datasets. Therefore, an efficient way to not only share these large datasets, but also allow for collaboration while processing these datasets, is necessary. To share these datasets across the NIST network, the NIST-developed Web Image Processing Pipeline (WIPP) system is used, which is an accessible and user-friendly system. The scripts that are used to generate these cell images are converted into a format that is suitable to be transferred with this system; a tool called Docker is utilized for this. We are using Docker to place these imaging scripts, the datasets, and any required libraries and software, into a virtual container, and these virtual containers can be accessed using the WIPP system. The development of these plugins will allow for users at NIST to process, analyze, view, and share large image datasets while minimizing the computational expertise required, which in turn provides an efficient way to not only process these large datasets but also for sharing and collaboration.



# SURF Student Colloquium

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August 1-3, 2023

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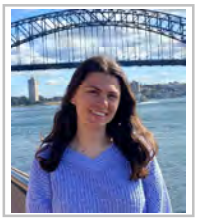
|---|---|---|---|
| **Name:** Sheetal Padhi | | | |
| **Academic Institution:** | New Jersey Insitute of Technology | **Major:** | Biomedical Engineering |
| **Academic Standing (Sept. 2023):** | Senior | | |
| **Future Plans (School/Career):** | Graduate School Pursuing a PhD in Biomedical Engineering | | |
| **NIST Laboratory, Division, and Group:** | Materials Measurement Lab Biosystems and Biomaterials Division, Cells System Science Group | | |
| **NIST Research Advisor:** | Dr. Anthony Asmar | | |
| **Title of Talk:** | Containerized Tools for Image Processing and Analysis of Live Induced Pluripotent Stem Cells | | |


**Abstract:**

With advancements in microscopy allowing for large scale imaging of induced pluripotent stem cells (iPSCs), sophisticated tools for processing and analysis are essential for biological research. iPSCs are unique in their ability to differentiate into specialized cells for use in therapeutics. They grow in colonies that are clumped together making it difficult to track individual cells using unlabeled imaging. A better understanding of how individual cells behave in the population by tracking is essential towards the development of better therapeutics. A Web Image Processing Pipeline (WIPP), developed at NIST, allows for the application of containerized tools for image processing and analysis of iPSCs while utilizing cluster computing resources. WIPP enables users to create open-source and customized workflows in order to process and analyze large datasets through a web-based platform. We are working on developing new plugins for WIPP to provide users access to advanced processing and analytical methods for the study of iPSCs. The advantage of using the WIPP system is due to its web-based interface; it allows these tools to be more accessible including ones to view large data with minimal computational and software resources on the user side. Developing WIPP plugins for iPSCs has multiple benefits such as promoting accessibility to imaging tools due to its web-interface format, fostering collaboration with its data viewing capabilities, and tracking image processing data and metadata to maintain provenance information.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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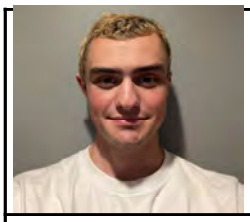
|---|---|
| **Name:** Carina DelCore | |
| **Academic Institution:** Georgetown University | **Major:** Chemistry |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | I plan to graduate with my B.S. and pursue a career in Environmental Chemistry research. |
| **NIST Laboratory, Division, and Group:** | Materials Measurement Laboratory, Biomolecular Measurement Division, Biomolecular Structure and Function Group |
| **NIST Research Advisor:** | Ella Mihailescu |
| **Title of Talk:** | An Investigation of Arginine-rich Antimicrobial Peptides and their Interactions with Lipid Membranes |


**Abstract:**

Antimicrobial peptides (AMPs) are a unique and diverse class of compounds that exhibit promising efficacy in terms of killing microbes. This is done through an attachment process, in which the amphipathic peptides can penetrate and interfere with the cell membrane to perform lysis, killing the cell. This property makes AMPs an intriguing prospect in the field of medicine. Arginine-rich peptides are an interesting subsect of the AMP group because they have a positive charge, which allows them to easily attract and interfere with the negatively charged and zwitterionic lipids often found in bacterial cell membranes. In this project, the Arginine-rich AMP building blocks R14, F5R8, and Cys-F4R8 were analyzed both in terms of their direct effects on live E. coli bacteria as well as their physical interactions with lipids (POPE, DMPC, and DPPG). This analysis was bolstered by investigation into the connection between amino acid sequences and AMPs' antimicrobial properties. The role of Cysteines was examined by creating dimeric AMP constructs via disulfide bond formation, which allowed for comparison of the reactivity and mechanics of an AMP dimer to those of the singular AMPs.

In order to better comprehend the bacterial cell destabilization that resulted from AMP introduction, techniques such as UV-Vis absorbance spectroscopy were applied to measure direct bacterial growth and death. By measuring the survival of E. coli in various concentrations, each AMP's minimum inhibitor concentration could be determined. Additionally, Differential Scanning Calorimetry analysis was applied to the lipid-AMP mixtures in order to observe the physical change that occurs upon AMP's introduction to the lipid bilayer. Furthermore, X-Ray Diffraction techniques were applied to model the lipid bilayer, so as to exhibit disruptions within it caused by the various AMPs. Overall, the objective of this project was to investigate anti-microbial peptides' effects on the bacterial cell membrane, as well as how these effects change with concentration and type of AMP. These observations will hopefully facilitate further research on AMPs as tools to fight bacterial infections and to reduce the overuse of conventional antibiotics.



# SURF Student Colloquium

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August 1-3, 2023

**Name:** Jonah Oxman

| **Academic Institution:** College of William & Mary | **Major:** Biology |
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**Academic Standing (Sept. 2023):** Junior

**Future Plans (School/Career):** Pursue a PhD in synthetic biology or microbiology

**NIST Laboratory, Division, and Group:** Material Measurement Lab, Biomolecular Measurement Division, Biomolecular Structure and Function Group

**NIST Research Advisor:** Dr. Curtis Meuse

**Title of Talk:** Characterizing Antibody Flexibility: 2D Codistribution Analysis of Disulfide Bond Reduction

**Abstract:**

Antibodies have quickly become a focus of the biopharmaceutical industry, spurred on by the recent pandemic. Monoclonal antibodies, such as the NISTmAb, consist of three subsections with two identical Fab domains and one Fc domain connected by a hinge region. The Fab domains contain the hypervariable regions that allow the antibody to bind to antigens. In this project, our focus is on learning more about the purpose of the hinge region, a flexible section of the protein, which contains disulfide bonds connecting the domains. Through a reduction reaction, these disulfide bonds can be broken to develop insight into the function of the hinge region. Raman spectroscopy has been previously used to analyze disulfide bond changes in albumin, chymotrypsin, and other cysteine polypeptide chains as they undergo reduction reactions. We employ IR spectroscopy and circular dichroism analysis to view the spectral changes as the reduction reaction occurs. By viewing bands in specific spectral regions, we can focus on the hinge region of the NISTmAb molecule to understand how water interacts with its amide bonds. Beginning with a technique known as 2D correlation analysis, we can investigate the different spectroscopic changes caused by the reduction reaction.While this spectroscopic information is useful in viewing reaction mechanisms, it does not always show the order in which the different reaction steps take place. 2D codistribution improves upon the 2D correlation by fitting the spectroscopic data with Lorentzian curves. Fitting the data can reduce noise in the analysis and allow us to better view the sequential order of the reaction steps. We hope to develop a fast and efficient method to separate the contributions of the domains from those of the hinge region of monoclonal antibodies. 2D codistribution analysis can be applied to other biomolecules to view how they might interact with water in newer biopharmaceuticals. Efficient methods for characterizing individual domain contributions can pave the way for the inclusion of a flexible section in smaller artificial antibody replacement drug molecules.

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August 1-3, 2023

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| **Name: Sragvi Pattanaik** | | |
| **Academic Institution:** | **University of Maryland, College Park** | **Major: Neurobiology and Physiology** |
| **Academic Standing (Sept. 2023):** | **Junior** | |
| **Future Plans (School/Career):** | **Medical School, Physician** | |
| **NIST Laboratory, Division, and Group:** | **MML Laboratory, Biosystems and Biomaterials Division, Complex Microbial Systems Group** | |
| **NIST Research Advisor:** | **Dr. Lisa Stabryla** | |
| **Title of Talk:** | **Exploring the Role of Bacterial Motility in Evolutionary Mechanisms for Antimicrobial Resistance** | |

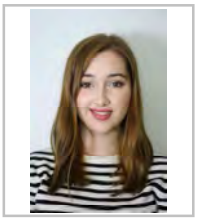

**Abstract:**

Antibiotic resistance (ABR) is the evolutionary response of bacteria to resist antibiotics intended to kill them. Pathogenic bacteria are especially problematic as they pose a greater clinical risk when resistant. Antibiotic resistance has become a major risk to human and environmental health as antibiotics are heavily relied on to overcome bacterial infection. To combat this issue, the scientific community works to find more rapid ways to identify antibiotic-resistant organisms, a critical step for treating bacterial infectious diseases.

Current microbiological methods of ABR detection include antimicrobial susceptibility testing (AST) (e.g., broth microdilution, and disk diffusion (Kirby-Bauer)). Such procedures are not considered rapid as they rely on multiple days of bacterial growth and monitoring. Molecular methods can be faster but are expensive, labor-intensive, and do not provide in-depth information about ABR profiles. However, identifying a commonly shared phenotypic marker (physical trait) of ABR, not limited by the growth rate, among bacterial strains could more rapidly detect ABR organisms.

Swimming motility is a conserved, observable trait across many bacterial species, making it a good candidate for a phenotypic marker. Thus, this project investigates the relationship between bacterial motility and the evolutionary resistance response to antibiotics in various clinically relevant organisms.

We will specifically study this relationship in two clinically relevant organisms: Uropathogenic *Escherichia coli* (UPEC) and Enterobacter spp. These bacterial strains are common causes of urinary tract infections and hospital-acquired infections. Their danger to public health is recognized by the CDC's urgent threat list of antibiotic-resistant organisms (i.e., the ESKAPE pathogens). Both strains are Gram-negative, rod-shaped, Enterobacteriaceae and use multiple flagella (hairlike threads along the cell body) that support free swimming. Flagella promote bacterial virulence and the capability to escape organismal immune response within human hosts. Our goal is to generate a suite of resistant bacteria in the lab using experimental evolution under sublethal exposure to common beta-lactam antibiotics (i.e., ampicillin and cephalexin). Strains will then be characterized for their resistance evolved alongside motility changes, measured using a swimming motility assay. Previous research with an environmental isolate of avian E. coli revealed a relationship between reduced swimming motility and evolved antibiotic resistance. Therefore, we hypothesize that this linkage will be generalizable to UPEC and Enterobacter spp, enabling faster detection of ABR in a wide variety of clinically relevant organisms.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Kira J. Corning |
| **Academic Institution:** | Saint Anselm College |
| **Major:** | Forensic Science |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Masters in Criminal Justice at Saint Anselm College with the hope of a future higher education on Forensic Anthropology |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory (MML), Materials Measurement Science Division (MMSD), Surface and Trace Chemical Analysis Group (MML 643.05) |
| **NIST Research Advisor:** | Briana Capistran |
| **Title of Talk:** | Generation of a Rapid GC-MS Library for Fire Debris Analysis and Ignitable Liquid Identifications |


**Abstract:**

Fire debris is one of the most common pieces of trace evidence scientists are tasked with analyzing in forensic investigations. The main objective when analyzing fire debris is to identify the presence or absence of ignitable liquid residues (ILRs). Ignitable liquids are often used to increase the spread and speed of a fire and can potentially indicate malicious intent when investigating an arson case. In the field of forensic science, gas chromatography-mass spectrometry (GC-MS ) is a widely accepted analytical technique used for the separation and detection of chemical compounds. Through this method, samples from a crime scene are extracted and analyzed using GC-MS to generate chromatograms and mass spectra. Sample chromatograms are visually compared to reference chromatograms of known ignitable liquids to identify liquids based on the compounds present. However, the instrumental analysis process takes time (~30 min/injection) and often creates backlogs in forensic laboratories. A newer technology, rapid GC-MS, is a screening technique that significantly reduces the time needed to analyze samples (~2 min/injection). The introduction of this instrumentation as a screening process to identify the presence or absence of ignitable liquids can eliminate the need for the long, traditional GC-MS analysis process, especially if the sample is absent of ILRs. Unfortunately, due to the recent development of this technique, reference chromatograms of known ignitable liquids are not available for rapid GC-MS. In this work, ignitable liquid samples were analyzed through rapid GC-MS to identify major compounds in each liquid and produce a series of known reference chromatograms. Total ion chromatograms (TICs) and relevant extracted ion profiles (EIPs) for all liquids were generated and included in the database. To test the utility of the reference database, data from blind samples and mock fire debris evidence were compared to the reference collection to identify the ignitable liquid present.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Nikhila Narayana |
| **Academic Institution:** | University of Colorado Boulder |
| **Major:** | Chemical Engineering/Music |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | I plan to work on renewable energy technology as a chemical engineer |
| **NIST Laboratory, Division, and Group:** | MML, Chemical Sciences Division, Chemical Process and Nuclear Measurements Group |
| **NIST Research Advisor:** | Dr. Donald Burgess |
| **Title of Talk:** | Compilation and Evaulation of Temperature Reference Points for the Alkali Metals |


**Abstract:**

We aim to compile and evaluate the melting and boiling points of the alkali metals. Many of these temperature values are already listed in chemistry handbooks, and researchers have written about many different methods used to calculate and measure these values. However, most of these sources do not provide uncertainties nor include citations to their original sources of data. In this work, we provide a comprehensive record of measurements found in open literature for the melting and boiling points of the alkali metals, as well as recommended values. Time permitting, we plan to compile and evaluate the vapor pressures used to determine boiling points and heats of vaporization.

In preparing this review, the key tasks include extracting data from available literature, exporting these values into a database, and preparing the data to input into a manuscript. In order to achieve this, we review abstracts and assess whether they contain relevant data using Web of Science, a platform containing citation data from many academic journals. After inserting these pertinent articles into EndNote, a reference manager, we collect the data from these articles and compile it in a database in Excel. In this database, we evaluate uncertainties, pressure ranges, and methods used to find these melting and boiling points. Where articles provide temperature and vapor pressure data, we graphically extrapolate the boiling points. Tables of this data are prepared for placing into a manuscript, and values are double-checked for accuracy. These tables reflect the temperatures provided in the original reference, as well as corrected values to reflect the current International Temperature Scale (ITS-90). Recommended values are provided by assessing values in the literature and selecting the most accurate values.

The melting points of the alkali metals Li, Na, K, Rb, Cs, and Fr are about 453.64±0.1 K, 370.944±0.005 K, 336.55 ±0.2 K, 312.65±0.1 K, 301.6±0.10 K, and 296±2 K, respectively. The boiling points of the the alkali metals Li, Na, K, Rb, and Cs are about 1613±2.0 K, 1156.09±0.005 K, 1031±1.0 K, 960±1.0 K, and 941.5±1.0, respectively. As can be seen, the temperature values consistently decrease with increasing atomic number, while the values for lithium are somewhat higher than the trends for the others.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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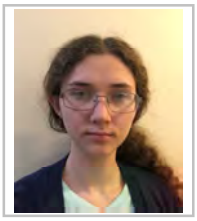
|---|---|
| **Name:** | Jacob Blinkoff |
| **Academic Institution:** | University of Maryland College Park |
| **Major:** | Chemical Engineering |
| **Academic Standing (Sept. 2022):** | Sophomore |
| **Future Plans (School/Career):** | Undecided |
| **NIST Laboratory, Division, and Group:** | Material Measurement Laboratory, Chemical sciences Division, Chemical Process and Nuclear Measurements Group |
| **NIST Research Advisor:** | Dr. Heather H. Chen-Mayer |
| **Title of Talk:** | Modeling Chloride Diffusion in Concrete |


**Abstract:**

Concrete is the most widely used building material in the world. Even so, it still has its weaknesses. An important issue surrounding concrete is the fact that it can suddenly and quickly lose its strength from corrosion. Rebar provides the tensile strength that concrete itself lacks, which makes it a much-needed addition when supporting large structures. When these steel rods corrode, depassivation via chloride oxidation tends to separate the steel rod into smaller sections, which greatly decreases its ability to provide support. Currently, the task of determining service life is performed by drilling a core from the structure for destructive chemical analysis. Nuclear techniques such as neutron capture prompt gamma analysis are being explored as a non-destructive alternative, which can be benefited by a numerical model of how chloride travels through a concrete medium.

This project investigates chloride diffusion in concrete using numerical simulation method, specifically looking at its relationship with aggregate structure. Typical diffusion modeling follows Fick's Laws, describing concentration as a function of depth with a constant diffusion coefficient. Due to concrete's complex pore/aggregate structure and chemistry, this diffusion constant can vary for the same formulations of concrete. To further try and refine this method of predicting chloride ingress, the channeling due to aggregate spacing and size will be considered. To estimate this, a COMSOL Multiphysics model for predicting the diffusion through the interior coarse aggregate given only a surface image of the concrete will be developed. The model will be based on a set of concrete cylinders of known composition and aggregate type, where the random aggregate distribution is represented as simple geometrical shapes. The model will be fitted to available concentration data to then be able to take any surface geometry and predict the chloride diffusion profile.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Sarah Lehrman |
| **Academic Institution:** | University of Maryland, Baltimore County |
| **Major:** | Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Graduate with Bachelor's Degree and pursue a career in Mechanical Engineering |
| **NIST Laboratory, Division, and Group:** | Material Measurement Lab, Materials Science and Engineering Division, Polymers Processing Group |
| **NIST Research Advisor:** | Stian Romberg |
| **Title of Talk:** | Determining the yield stress and frequency dependence of printable thermoset composite resins |


**Abstract:**

For successful thermoset resin additive manufacturing, the material must have a low enough viscosity to flow when being deposited, but also be strong enough to hold its shape so the curing process can occur. This is an issue because neat thermoset resins cannot support their own weight, allowing prints to deform or collapse before curing can fully solidify the resin. Addition of fillers, such as fumed silica, creates a gelled thermoset composite with a yield stress that can mitigate this instability while still allowing the material to flow during extrusion. Rheology, the study of the flow and deformation of matter, can be utilized to determine the amount of filler required to gel the thermoset composites and measure the associated yield stress.

In this study, samples of epoxy resin (EPON 826) are mixed with an amine curing agent (JEFFAMINE D-230) and varying quantities of fumed silica (CAB-O-SIL TS-720). Each sample is loaded into a rheometer to undergo a strain amplitude sweep. This test determines how the yield stress varies for different amounts of fumed silica. It also determines the linear viscoelastic region (LVR) in order to understand the strain at which a frequency sweep could be conducted. The subsequent frequency sweep tests help determine the fumed silica content that causes the composite to gel. Novel "chirp" measurements are also conducted and compared to the traditional frequency sweep results. These "chirp" measurements test a range of frequencies virtually instantaneously, which is important for fast-curing thermoset composites whose properties can change faster than traditional frequency sweep measurements can be conducted. This data is then exported from the rheometer software and read using MATLAB for review and analysis. All of this is done to understand the rheological signature of printed composites and ensure that "chirp" measurements match frequency sweep measurements.

# NIST Center for Neutron Research 2023

**Summer Undergraduate Research Fellowship (SURF) - 2023 Participants**

*(in the order of the Colloquium schedule)*

NIST Center for Neutron Research (NCNR)

***Ethan Gasper:*** Effects of solvents on the assembly of nanoparticles from poly(styrene-b-ethylene glycol)

*Patrick Chen:* Simulating Domain Walls in Weyl Semimetals to Study the Effects of Weyl Fermions on Magnetic Behavior

*Kimia Samieinejad:* Chemical Vapor Deposition of Uranium Ditelluride (UTe2)

*Justin Wang:* Reinforcement Learning and Spin Waves

*Navid Misaghian:* Harmonizing Human-Machine Interfaces: A Standard Reference Guide for HMI Design and Management at the NCNR

*Amir Dajani:* Development of a Validated CFD Model for the Mixing Behavior of Parallel Triple

*Kaitlyn Esneault:* Sample Development for Small Angle Scattering and Neutron Interferometry

*Sanjana Sureshbabu:* Constructing Native Extracellular Scaffolds for Tissue Repair

*Surabhi Singh:* Understanding Mitochondrial Dysfunction Through Structures of Cardiolipin Cytochrome c in Healthy and Pathological Model Membranes

*Rahil Verma:* Optimizing Pharmaceutical Formulations

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Ethan Gasper | |
| **Academic Institution:** George Mason University | **Major:** Chemistry |
| **Academic Standing (Sept. 2022):** | Sophomore |
| **Future Plans (School/Career):** | Graduate from GMU and possibly pursue a Master's in Chemical Engineering |
| **NIST Laboratory, Division, and Group:** | NIST Center for Neutron Research (NCNR), Neutron-Condensed Matter Science Group |
| **NIST Research Advisor:** | Kelsi Rehmann and Katie Weigandt |
| **Title of Talk:** | Effects of solvents on the assembly of nanoparticles from poly(styrene-b-ethylene glycol) |


**Abstract:**

Block copolymers can form many different structures based on interactions between the polymers blocks and solvent. We will study different processes of making spherical core-shell nanoparticles with water and tetrahydrofuran (THF), where one polymer acts as an outer shell and the other acts as the inner core of the sphere. We are testing how different solvents, varying mixing methods of copolymers, and purification processes of nanoparticles affect the self-assembly of core-shell nanoparticles produced from poly(styrene-b-ethylene glycol) (PS-b-PEG) block copolymers. The main synthesis process to create nanoparticles involves mixing two PS-b-PEG polymers, where the polystyrene block have different molecular weights, and adding the mixture into THF solvent. Water is slowly added to initiate the self-assembly of the nanoparticles, then the solution is added to an ultrafiltration device to isolate the nanoparticles in the water. By changing the ratio of molecular weight of polystyrene core, we will change the structure of the nanoparticles, because the interactions between the solvent and polymers change to result in different structures and different densities of the core and surface polymers of the nanoparticles. To understand the changes between each method, we use small angle scattering (SAS) and dynamic light scattering (DLS) to determine the core radius and the hydrodynamic radius of the nanoparticles, respectively. The structure of the PS-b-PEG nanoparticles can be determined from the information provided by SAS and DLS, as well as how the size and structure of the nanoparticles change in response to different processing methods, different solvents that dissolve the copolymers, and changes in the molecular weight of copolymers.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|---|
| **Name:** Patrick Chen | | | |
| **Academic Institution:** | University of Maryland -College Park | **Major:** | Physics and Math |
| **Academic Standing (Sept. 2023):** | Junior | | |
| **Future Plans (School/Career):** | Graduate School | | |
| **NIST Laboratory, Division, and Group:** | NCNR | | |
| **NIST Research Advisor:** | Jonathan Gaudet | | |
| **Title of Talk:** | Simulating Domain Walls in Weyl Semimetals to Study the Effects of Weyl Fermions on Magnetic Behavior | | |


**Abstract:**

The electrons within the atoms of magnetic materials have an inherent property called spin, which allows each atom to be thought of as a tiny magnet. The alignment of the spins throughout a material determines its macroscopic properties. Regions of aligned spins are called domains, and there can often be many domains with different alignments of spin within the same material. In such a scenario, there exist domain wall regions between the domains where the spins transition from one alignment to the other. The behavior of the spins within this region are determined by the interactions between them, which we here focus on the ones mediated by conductive Weyl electrons. Weyl electrons are massless chiral particles that have been recently found to emerge in specific materials. The chirality of the Weyl electrons is theoretically predicted to induce bond-dependent Dzyaloshinskii-Moriya (DM) interactions between spins of a material. Thus, we performed micro-magnetic simulations of domain walls including the effect of bond-dependent DM to study the predicted effects of Weyl electrons. These simulations based in theory can then be compared to small-angle neutron scattering(SANS) data of candidate magnetic Weyl semimetals.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Kimia Samieinejad |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Physics and Computer Science |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate School |
| **NIST Laboratory, Division, and Group:** | NIST Center for Neutron Research, Neutron Condensed Matter Science Group |
| **NIST Research Advisor:** | Nick Butch |
| **Title of Talk:** | Chemical Vapor Deposition of Uranium Ditelluride (UTe2) |


**Abstract:**

Chemical Vapor Deposition (CVD) is a crucial technique for fabricating high-quality thin films by depositing gaseous reactants onto a substrate. This research project focuses on creating and testing an apparatus for synthesizing UTe2 films using CVD. UTe2 exhibits intriguing physical properties, including superconductivity, topological behavior, and potential exotic states. By leveraging CVD, we can precisely control the deposition process and obtain high-quality UTe2 films for detailed characterization.

This project also involves theoretical simulations that analyze and predict various aspects of the deposition process. These simulations encompass intermediate reaction steps, potential by-products, reaction mechanisms, and the stoichiometry of the deposit. This research project combines theoretical analysis, experimental synthesis, and exhaustive scrutiny to explore the chemical vapor deposition of UTe2 films.

I will discuss the insights gained from theoretical simulations and my testing of the experimental setup.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Justin Wang | |
| **Academic Institution:** Johns Hopkins University | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Graduate School (PhD) |
| **NIST Laboratory, Division, and Group:** | NCNR |
| **NIST Research Advisor:** | William Ratcliff |
| **Title of Talk:** | Reinforcement Learning and Spin Waves |


**Abstract:**

Neutron scattering is a powerful tool, with uses such as probing crystal structures and estimating magnetic order parameters. However, as there are a very limited number of neutron sources in the world, it's difficult to have access to neutron beams, so it's important to execute experiments as efficiently as possible.

This project builds on previous student work, exploring the idea of applying reinforcement learning to optimize neutron scattering experimental time. It focuses specifically on spin waves, which are created by exciting the magnetic structure within a crystal lattice with neutrons. The MATLAB implementation SpinW is used to model these spin waves; some of its functions include generating predefined spin Hamiltonians (used to approximate energy), calculating spin wave dispersion, and plotting.

Experimental optimization has been approached in the community using Bayesian Optimization (Active learning), and former students on the project attempted the problem using an Actor-Critic RL algorithm. This project will approach from yet another angle using a different RL algorithm, Q-learning, to allow for better offline training of the algorithm. We also attempt to improve the translation of MATLAB code of SpinW into Python. This will extend the previous work by allowing us to model not only the spin wave dispersion, but the neutron intensities as well.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Navid Misaghian |
| **Academic Institution:** | University of Maryland College Park |
| **Major:** | Computer Science & CIS |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Software Engineering (Full Stack Development or Machine Learning) |
| **NIST Laboratory, Division, and Group:** | NCNR |
| **NIST Research Advisor:** | Whipple, James and Newby, Robert |
| **Title of Talk:** | "Harmonizing Human-Machine Interfaces: A Standard Reference Guide for HMI Design and Management at NCNR" |


**Abstract:**

The National Institute of Standards and Technology's Center for Neutron Research (NCNR) houses a diverse array of complex human-machine interfaces (HMIs), each distinguished by unique color schemes, designs, and structures. This project's primary objective is to develop a comprehensive standard reference guide for future HMI implementations within the NCNR. Well-structured HMIs are instrumental in decreasing training time, curtailing startup or shutdown durations, and minimizing any uncertainties associated with machine interfaces. This initiative aims to bolster consistency, ease of use, and boost operational efficiency across the center's machinery.

To streamline this project, we leverage key industry standards from diverse sources, including ISA, ANSI, and HFES. These guidelines shape our approach towards usability and performance, enabling us to tailor our standard guide to meet the varied and diverse needs of the NCNR's user base. This project emphasizes the crucial role of trained human factors engineers in implementing and assessing these specifications.

By assessing insights from these references with existing practices at NCNR, our aim is to create a reference guide encapsulating the best principles of HMI design and management. Ultimately, this project will enhance machine interactions at NCNR, establishing a foundation for improved user experiences, a unified design aesthetic, and streamlined operations.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Amir Dajani

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

**Academic Standing (Sept. 2023):** Senior


**Future Plans (School/Career):** Join industry as a Bioengineer, with a focus on the engineering and design aspect. Additionally, pursue higher education, either in a Computational field or an MBA.


**NIST Laboratory, Division, and Group:** NCNR

**NIST Research Advisor:** Abdullah Weiss


**Title of Talk:** Development of a Validated CFD Model for the Mixing Behavior of Parallel Triple-Channel Flows


**Abstract:**

Computational Fluid Dynamics (CFD) models provide information regarding how fluids and their flow interact with different environments. The study at hand specifically focuses on a triple-channel mixing flow in a confined channel, producing similar behavior to flows in the inlet of the pre-conceptual design of the NIST Neutron Source (NNS), which seeks to replace the existing reactor at NCNR. The NNS inlet forces the coolant to split into three different legs, after which they mix again, thus causing a separation-mix pattern that is found in triple channel flow mixing studies. In order to model this flow, a geometry of the mesh, which represents a reference experiment's test section, must first be created. OpenFOAM is a CFD software that has this capability and is thus used in constructing the mesh. Once the mesh is created, different turbulence models, like k-$\epsilon$ and k- $\omega$, are then used to model the flow. The values for certain variables, like velocity and pressure, specific to each model type are adjusted and the simulation is then run. Contour and line plots are used to study the flow's behavior and it is then used to compare to results from literature. The comparison to literature enables the validation of the CFD model and the selection of an appropriate turbulence model. Such validation would help ongoing efforts to characterize the flow behavior at the inlet of the NNS.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|
| **Name:** Kaitlyn Esneault | | |
| **Academic Institution:** Rice University | **Major:** Chemical and Biomolecular Engineering | |
| **Academic Standing (Sept. 2023):** | Senior | |
| **Future Plans (School/Career):** | Professional Master's degree and/or industry work | |
| **NIST Laboratory, Division, and Group:** | NIST Center for Neutron Research, Neutron-Condensed Matter Science Group | |
| **NIST Research Advisor:** | Caitlyn Wolf, Katie Weigandt | |
| **Title of Talk:** | Sample Development for Small Angle Scattering and Neutron Interferometry | |


**Abstract:**

Small angle scattering (SAS) is a technique that has long been used to gather structural information about materials at small length scales, from 1 nm to 10 μm. However, results are sample-averaged, so the method has proved difficult to use for complex, heterogeneous, or hierarchical samples. INFER, a novel neutron far field interferometer under development at the NIST Center for Neutron Research, attempts to address this issue by gathering structural data at multiple length scales simultaneously. The instrument uses dark field imaging to produce spatially resolved images where each pixel captures structural information at the same length scales currently probed by SAS. This dark field intensity data can be simulated by applying a Hankel transform to SAS data. Ongoing research is validating the accuracy of both experimental INFER data and SAS-based simulations with samples of monodisperse, spherical polystyrene nanoparticles. However, to probe further into INFER's limitations and capabilities, as instrument development advances, we aim to increase the complexity of the materials used to test it. In my research, I use a self-assembling surfactant-cyclodextrin complex to develop a more elaborate validation sample series. At varying concentrations in aqueous solution, the complex assembles into different supramolecular structures: lamellae, microtubes, or polyhedra. Using a combination of dynamic light scattering (DLS) and SAS for characterization, my experiments explore the phases of this system not only across a spectrum of concentrations, but also with different temperatures and combinations of cyclodextrins and surfactants. Future research can use this data to validate measurements from INFER, confirming the continued accuracy of both the Hankel transform model and the instrument itself, and ultimately supporting the instrument's use in characterizing heterogeneous samples.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Sanjana Sureshbabu |
| **Academic Institution:** | American University |
| **Major:** | Biochemistry and Data Science |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Graduate School |
| **NIST Laboratory, Division, and Group:** | NCNR |
| **NIST Research Advisor:** | Minh Phan |
| **Title of Talk:** | Constructing Native Extracellular Scaffolds for Tissue Repair |


**Abstract:**

Biocompatible polymers and tissue-derived scaffolds are commonly used in clinics for tissue repairs. However, these come with complications. Non-native polymers often fail to produce cell-cell communication, while native scaffolds from tissues have risks of disease transmission and immunological rejection due to incomplete cell removal. Cell-derived extracellular matrix (ECM) overcomes those obstacles, but the low-yield ECM production limits its advancements in clinical applications. In this project, we aim to engineer ECM pre-scaffolds that match cell requirements and to feed them into the cell culture to facilitate the ECM production process. We utilize lipid membranes to unfold proteins and make them ready to assemble into larger structures. The pre-scaffolds comprise single or multiple ECM's key components, including collagen type I, elastin, fibronectin, and laminin. Langmuir isotherms, adsorption assays, and X-ray reflectometry will elucidate the membrane's physical properties and capture detailed structures of the pre-scaffolds forming on the membrane surface. These results will create a comprehensive knowledge of ECM nanoscopic fibrillar textures that would guide future ECM-mimetic material development in the tissue engineering community.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Surabhi Singh |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Bioengineering |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | Graduate School, followed up with industry work prosthetics and medical devices development |
| **NIST Laboratory, Division, and Group:** | NIST Center for Neutron Research (NCNR), Neutron-Condensed Matter Science Group |
| **NIST Research Advisor:** | Dr. Minh Phan |
| **Title of Talk:** | Understand Mitochondrial Dysfunction Through Structures of Cardiolipin-Bound Cytochrome c in Healthy and Pathological Model Membranes |


**Abstract:**

Cardiolipin (CL) is a unique phospholipid that helps regulate protein binding and integration into the inner mitochondrial membrane (IMM). Cytochrome c (Cytc) is a protein that assists the electron transport chain and is anchored to the IMM by CL. Alteration of CL's concentration and chemical structures due to the malfunction of internal lipid synthetic pathways leads to diseased mitochondria and potentially shuts down ATP production. This occurrence leads to the progression of bioenergetic diseases.

This summer, I developed various CL-containing model membranes to mimic the real IMM using known healthy and diseased forms of CL and investigated how certain CL changes regulate Cytc binding to the film. The CL-containing membrane and Cytc interfacial interaction will be thoroughly elucidated by Langmuir isotherms and in situ X-ray reflectometry, where insights into CL effects on the physical properties of the membrane and how they regulate Cytc's binding structure will be captured. These results would reveal the underlying mechanism of the corresponding mitochondrial conditions.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Rahil Verma |
| **Academic Institution:** | Duke University |
| **Major:** | Biomedical Engineering |
| **Academic Standing (Sept. 2023):** | Sophomore (2nd year) |
| **Future Plans (School/Career):** | Biomedical Engineering industry, prosthetics, medical devices, consulting |
| **NIST Laboratory, Division, and Group:** | NCNR (NIST Center for Neutron Research) |
| **NIST Research Advisor:** | Rachel Ford |
| **Title of Talk:** | Optimizing Pharmaceutical Formulations |

**Abstract:**

Pharmaceutical drug formulations include the active drug protein, preservatives, and surfactants among other components. Typically surfactants such as poloxamer 188 and polysorbate 80 are used to keep active drug proteins evenly dispersed in solution, while preservatives such as benzyl alcohol and phenol are used to prevent microbial growth in formulations. An optimal formulation maximizes the antimicrobial strength of preservatives while remaining evenly dispersed in solution and staying within the pharmaceutical limits. While the solubility limits for these components are well above the pharmaceutical limits on their own, aggregation is observed when surfactants and preservatives interact in solution. In this study, the formation of turbid aggregates was observed in compositions including poloxamer 188, polysorbate 80, benzyl alcohol, and phenol. The turbidity boundaries for formulations were explored by creating phase diagrams at varying conditions, with phases observed as either clear or turbid. Turbidity indicates the formulation is no longer evenly dispersed and consequently unstable. In addition to observing surfactants and preservatives, bovine serum albumin was used as a model protein to infer the effects of a typical active drug protein on the turbidity boundary. Dynamic light scattering (DLS) was also used to determine the mechanism by which aggregation occurs, indicating how to better prevent turbidity in formulations. By investigating the relationship between composition, temperature, and turbidity, stable ranges of concentrations for these excipients can be provided for pharmaceutical use.


# Physical Measurement Laboratory 2023

**Summer Undergraduate Research Fellowship (SURF) - 2023 Participants**

*(in the order of the Colloquium schedule)*

Physical Measurement Laboratory (PML)

*Seoyoung Joo:* A real and k-space imaging spectroscopy setup for nanophotonic device characterization

*Jacques Deroin:* COMSOL Simulations of Electromagnetic Test Structures

*Daniel Harrington:* Polymer Passivation of 2D TMD Photodetectors

*Jarlem Lopez Morel:* Organic Electrochemical Transistors with a Gold Nanoparticle-Doped Polymer Channel

*Audrey Pechilis:* Transient Absorption Spectroscopy of Exciton-Polaritons in Organic Crystals

*Nathaniel Lawson:* Advanced charge pumping techniques for defect detection and characterization in MOSFETs

*Benjamin Tran:* DC Power and Energy Calibrations to Verify Electric Vehicle Supply Equipment Meters

*Bryan Rezende:* Development of the calibration service for level 3 direct current (DC) power energy meters

*Andrew Peters:* The Missing Link: Automation of Magneto-Optical Spectroscopy of Quantum Materials

*Brady Egleston:* Characterizing 39K MOT clouds with Neural Networks

*Noah Zuckman:* Analysis of test data from the
portable EBIT for NIST Boulder

*Joshua Young:* Development of an Ultrasonic Calorimeter for Dose Rate Imaging

*Alisha Patel:* Analyzing the Effects of V-Vial Parameter Changes on Ionization Chamber Response Using TOPAS

*Ethan Zheng: The modelling and testing of the Wide Angle Free Air Chamber*

*Travis White:* Analyses in Laboratory Metrology

*Dinelka Jagoda:* Educational Outreach Resources

*Jeremy Robin:* Multiplexed Electrochemical Biosensing

*Ginny McCracken:* Fabrication and Characterization of Functionalized Graphene Field Effect Transistor for the Quantification of Exosomes Produced by Induced Pluripotent Stem Cell-Derived Cardiomyocytes

*Connor Skelton:* Uncertainty Quantification in Flow Cytometry with AM Modulation *Olivia Green:* Testing the performance of optomechanical pressure sensors

*Benjamin Baldwin:* Rotational Cooling of a Molecular Beam

*Gabriel Kuntz:* Developing a robust and cost-effective digital PID controller for laser cooling

*Grace Waters:* Measuring the Bidirectional Reflectance of Materials for UVC Germicidal Applications

*Rishabh Sinha:* Simulation and Measurement of 3D Thermal Gradients in Liquids for Magnetic Imaging Validation

*Dawn Pierce:* Measuring the UV Transmittance of DMDs and How It Will Help Us Search for Habitable Exoplanets

*Briana Chen:* Measuring digital micromirror device characteristics in the infrared wavelength regime

*Colleen Ewald:* Impact of the Degradation rate of Photodiodes on CANDLE Project

*Amanda Younes:* Rydberg atom sensing of blackbody radiation

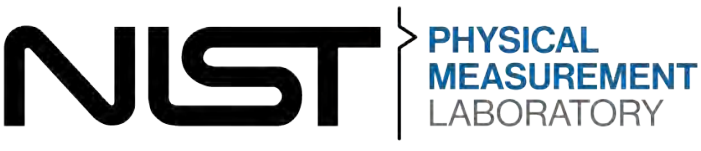
*Addhyaya Sharma:* Assembling DNA origami fused plasmonic nanopores for single molecule detection

*Ziran Du:* Saturation of Susceptibility in a Two-Level System, a Model of a Rb Vapor Cell

*John Taylor:* Examining the Experimental Limitations of the Quantum Ampere

*Mya Merritt:* Obtaining Super Resolution with Thermal States using Photon Number Resolving Camera

*Justin Craven:* Faster ultracold atom data collection through the use of a one-dimensional optical molasses



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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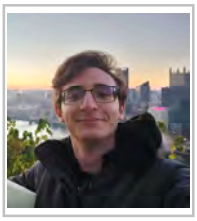
|---|---|
| **Name:** | Seoyoung Joo |
| **Academic Institution:** | Carnegie Mellon University |
| **Major:** | Materials Science and Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | PhD in Materials Science and Engineering |
| **NIST Laboratory, Division, and Group:** | PML, Microsystems and Nanotechnology Division, Photonics and Optomechanics Group |
| **NIST Research Advisor:** | Amit Agrawal |
| **Title of Talk:** | A real and k-space imaging spectroscopy setup for nanophotonic device characterization |


**Abstract:**

Fourier microscopy is an increasingly important tool for use in the analysis of optical nanostructures, as it measures the energy and angle of outgoing light from a given device. However, most optical microscope configurations have been optimized for conventional real-space imaging. Thus the impact of design choices made in such imaging, such as aberrations, must be re-analyzed and accounted for when reconfiguring for Fourier microscopy.

We designed an optical microscope that allows for real-space and Fourier-space imaging and spectroscopy of a sample. The real-space configuration relays the image formed by a commercial microscope onto the input of a spectrometer, while the Fourier-space configuration relays the back-focal plane to the same spectrometer input. The design allows for rapid switching between the two configurations. We showcase our setup by imaging a set of plasmonic gratings, as well as other photonic devices, and by measuring real-space and Fourier-space transmission spectra of these devices.



# SURF Student Colloquium

NIST – Gaithersburg, MD

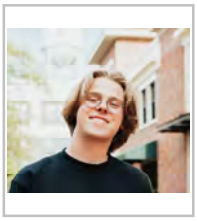
August 1-3, 2023

| | |
|---|---|
| **Name:** | Jacques Deroin |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Chemistry |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate school<br>Career in physical/nuclear chemistry |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Nanoscale Device Characterization Division, Advanced Electronics Group |
| **NIST Research Advisor:** | Yaw Obeng, Joseph Kopanski |
| **Title of Talk:** | COMSOL Simulations of Electromagnetic Test Structures |


**Abstract:**

As the amount of data handled by electronic systems increases over time, the ability to transmit signals at ever higher speeds is crucial. This demand has led to the development of 3D integrated circuits (3D-ICs), where chips are stacked vertically to ensure an optimal balance between speed and power consumption.

At high temperatures, copper diffuses into dielectrics, causing degradation of the circuit. This presents a need for a cladding layer between the copper line and the dielectric layer. Typically, these barriers are constructed from tantalum compounds. This project aims to explore novel materials for copper interconnect cladding by evaluating the impact of novel copper barrier candidate materials on high speed signal loss. Broadband dielectric spectroscopy (BDS) has been used to measure signal loss (S-parameter) as a function of the dielectric properties of cladding materials. This project is a continuation of a previous SURF project's work (Jesus Perez, 2019) by expanding the range of materials studied to WSxSe2-x. A microstrip model has been created in the COMSOL multiphysics FEM software and simulations of cladding materials are currently underway. These simulations will provide valuable insight into the impact of the material composition and chemistry on the dielectric constant.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|
| **Name:** Daniel Harrington | | |
| **Academic Institution:** Tufts University | **Major:** Physics, Mathematics | |
| **Academic Standing (Sept. 2023):** | Sophomore | |
| **Future Plans (School/Career):** | Pursue a PhD in physics and a career in research | |
| **NIST Laboratory, Division, and Group:** | PML, Nanoscale Device Characterization Division, Nanoscale Spectroscopy Group | |
| **NIST Research Advisor:** | Dr. Christine McGinn, Dr. Christina Hacker | |
| **Title of Talk:** | Polymer Passivation of 2D TMD Photodetectors | |


**Abstract:**

In recent years, 2D transition metal dichalcogenides (TMDs) have demonstrated optoelectronic properties that make them interesting for photodetectors and other semiconductor applications. Among the most studied is molybdenum disulfide (MoS2), which in its monolayer structure is a direct bandgap semiconductor. Several works have examined performance of MoS2 photodetectors in various device configurations, including in heterostructures with other 2D materials and with ferroelectric polymer poling to improve detectivity and other figures of merit. Here we investigate the passivation effects of various polymers on the performance of FET MoS2 photodetectors.

We examined samples with CVD-grown MoS2 on sapphire substrate. Samples were coated with one of PMMA, Parylene-N, or P(VDF-TrFE), and their properties were compared. Initial characterization methods were Raman spectroscopy and hyperspectral photoluminescence (PL) imaging. We then used THz time domain and time resolved spectroscopy to determine sample photoconductivity and compare charge recombination and mobility. We then fabricated devices with exfoliated MoS2 on SiO2/Si substrate and will be comparing device performance to investigate a change in performance across the polymer coated devices.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Jarlem M. Lopez Morel |
| **Academic Institution:** | Wake Forest University |
| **Major:** | Physics, BS |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Physics Graduate School; HS science teacher |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory<br>Nanoscale Device Characterization Division - Nanoscale Spectroscopy Group |
| **NIST Research Advisor:** | Dr. Katelyn Goetz and Dr. Emily Bittle |
| **Title of Talk:** | Organic Electrochemical Transistors with a Gold Nanoparticle-Doped Polymer Channel |


**Abstract:**

In modern electronics memory and computation are built into separate circuit elements. Memory is often stored in magnetic elements and computation is done by electrical switches called transistors. By combining computation and memory, electronics may be made more compact and energy efficient. Electrochemical transistors are transistors in which the switching voltage is applied through an electrolyte. That is, the current that flows through the device's source and drain contacts is controlled by the exchange of ions of an electrolyte with the channel that connects these contacts. This channel is made up of a conductive or semiconductive material. The channel material can be implanted with particles that can trap and release charge or ions during operation, creating a dynamic memory within a transistor, and effectively opening the possibility of combining memory and computation into the same element.

Our project investigates the impact of adding gold nanoparticles to the channel material in organic electrochemical transistors (OECTs) which has shown promise as a memory transistor with mechanical flexibility and bio-compatibility common to organic electronics. The channel material we use is the polymer poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS). This is a very efficient material for organic transistors: it is highly conductive, and it has a lower cost of processing than other widely used materials like silicon, giving it the added benefit of affordability. We are focusing on seeing how the gold nanoparticles impact the transistor switching characteristics, that is, the relation between the voltage going through the electrolyte and the drain-source current. Analyzing how PEDOT:PSS channels with varying concentrations and sizes of gold nanoparticles impact the functioning of OECTs would allow us to obtain guidance on how to improve the performance of this material for future memory-computing applications.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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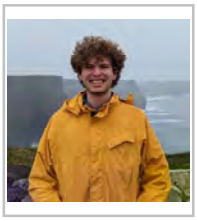
|---|---|
| **Name:** | Audrey Pechilis |
| **Academic Institution:** | University of California Santa Barbara |
| **Major:** | Physics |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | PhD in Particle Physics |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Nanoscale Device Characterization Division, Nanoscale Spectroscopy Group |
| **NIST Research Advisor:** | Jared Wahlstrand |
| **Title of Talk:** | Transient Absorption Spectroscopy of Exciton-Polaritons in Organic Crystals |


**Abstract:**

In transient absorption spectroscopy experiments, the energies that reside in a molecular sample are detected using a series of two lasers. The first laser excites the electrons to a higher energy state, and when another laser passes through, the laser's spectrum is intermittently absorbed at the wavelengths corresponding to the energy levels of the electrons. By subtracting the spectrum of the unexcited ground state from the spectrum of electrons excited to higher energy states, the existing energy states of the molecule can be detected at varying time delays between excitation and absorption. This technique allows for signal detection at very small time scales which resolves the intermediary transitions between decays. On such a short time frame, however, the phase difference between the short and long wavelengths of the beam becomes a confounding factor in data interpretation because absorption in the second pulse does not all happen at the same time. To correct for this phase difference across wavelengths, we have put together a pulse shaper which allows us to separate the wavelengths, electronically adjust the phase of each wavelength via liquid crystal orientation, and recombine the wavelengths into a condensed beam.

This technique allows for signal detection at very small time scales and track the movement of energy between states in molecular compounds before they decay back to the ground state. Tetracene is a crystal in which, like many organics, the electron-hole pair created by excitation can undergo fission into a polariton. This split energy state is composed of a higher and a lower energy state, the latter of which can decay further into a triplet energy state. The triplet state is essentially an excited state at half the energy of the lowest singlet excited state, which significantly broadens the scope of tetracene's applicability. Since the triplet state in tetracene matches the singlet state in silicon, the integration of a tetracene component could for example double the energy intake of solar cells.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|---|
| **Name:** Win Lawson | | |
| **Academic Institution:** University of Illinois Urbana-Champaign | | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Graduating December 2023 | |
| **Future Plans (School/Career):** | I will apply for grad school and I aim to pursue physics research relevant to improving computer hardware. | |
| **NIST Laboratory, Division, and Group:** | PML, Nanoscale Device Characterization Devision, Alternative Computing Group | |
| **NIST Research Advisor:** | Jason Ryan, Stephen Moxim | |
| **Title of Talk:** | Advanced charge pumping techniques for defect detection and characterization in MOSFETs | |


**Abstract:**

The widespread adoption of metal oxide semiconductor field effect transistors (MOSFETs) has prompted the development of advanced characterization methods of said devices. A specific quantity of interest is how many atomic scale defects exist in a particular device. In MOSFETs, differing lattice structures between the semiconductor and oxide leave some bonds unsatisfied at the interface between the two materials. These unsatisfied bonds (or defects) have the ability to capture electrons and by extension impact the electronic properties of devices, which have little tolerance for error. One method for determining defect density is known as charge pumping (CP).

In CP a transistor is configured such that when a square wave voltage is applied to the gate, a recombination current can be measured through the substrate. The measured current is proportional to the defect density as well as the frequency of the square wave, and can be used to "count" the defects. The technique has been used extensively in research and industry, and several advancements have allowed CP to be used even in highly-scaled MOSFETs. Other efforts have been made to extract more information from the response aside from just defect density.

This talk will discuss two advanced CP techniques. Frequency modulated CP (FMCP) can be used to eliminate leakage currents which obscure the CP response. While CP current is proportional to frequency, leakage current is not, so when the CP frequency is modulated and the signal is examined using a lock-in amplifier, the CP current is amplified but the leakage is not. A second technique known as spin-dependent CP (SDCP) incorporates electron spin resonance into the CP detection. The resulting response can be interpreted to give chemical and physical information about the defects themselves. The potential combination of FMCP and SDCP will also be discussed. Successful FM SDCP would be instrumental in making further improvements in state-of-the-art integrated circuits, and could aid in the development of a CP-based quantized current source.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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| **Name:** | Benjamin Thanh-Sang Tran |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Electrical Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Career in Electrical Engineering/Information Technology |
| **NIST Laboratory, Division, and Group:** | Physical Measurements Lab, Office of Weights and Measurements |
| **NIST Research Advisor:** | Dr. Maritoni Litorja |
| **Title of Talk:** | DC Power and Energy Calibrations to Verify Electric Vehicle Supply Equipment Meters |


**Abstract:**

The Level 3 electric vehicle (EV) charging station, also known as electric vehicle supply equipment (EVSE), is the latest form of EV charging. These direct current fast-charging (DCFC) charging stations are significantly more powerful and faster than previous versions due to their ability to convert higher levels of alternating current (AC) voltage directly from the grid into direct current (DC) voltage internally before fueling an EV's batteries. External field meters are needed by state regulators to measure and verify the output power and energy of installed DCFCs. The secondary field meters used during these inspection services must be calibrated to be traceable to the SI in order to render confidence in the commercial transactions. Within the Applied Electrical Metrology lab at NIST, we simulated the voltage and current of a Level 3 EV charging station using research-grade sources and then measured its voltage, current, power, and energy outputs using calibrated multimeters throughout the simulation in LabVIEW. User interface modules and post-acquisition data analysis modules for calibrating were then generated. I designed a virtual instrument (VI) in LabVIEW that pulled the electrical quantities and specifications from the simulation VI, processed and organized the data, and outputted it as a .csv and .txt for further analysis. A preset feature was also implemented into the simulation VI to allow for graphical replication of the nature of the EV battery charging duration.

Most current commercial charging stations are Level 2 EVSEs that must undergo inspections in order to verify that they are outputting the energy in kW-h that a customer is billed for. I participated in a Level 2 AC EV charging station mock inspection with the Office of Weights and Measurements (OWM) using the Examination Procedure Outline (EPO 30), the guidance document that state inspectors follow to check commercial EVSEs. The inspection included verifying that the charging station is in compliance with the specifications, tolerances and other technical requirements of Electric Vehicle Fueling Systems according to NIST Handbook 44 Section 3.40.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Bryan F. Rezende |
| **Academic Institution:** | University of Maryland, College Park |
| **Major:** | Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Physics research in quantum sensing |
| **NIST Laboratory, Division, and Group:** | PML, Quantum Measurement Division, Applied Electrical Metrology Group |
| **NIST Research Advisor:** | Richard L. Steiner |
| **Title of Talk:** | Development of the calibration service for level 3 direct current (DC) power energy meters |


**Abstract:**

Though the National Institute of Standards and Technology (NIST) has developed and published standards for level 1 and level 2 electric vehicle supply equipment (EVSE) utilizing alternating current (AC) power, we are currently in the development phase for prescribing standards to the level 3 systems utilizing direct current (DC) power. State agencies regulating weights and measures and industry calibration laboratories will depend on NIST's development of level 3 charging calibration services in order to certify traceability to SI units and the accuracy of transactions involving these chargers. My work consists of several elements that aim to develop integral parts of such a service.

An instrumentation rack composed of digital multimeters (DMMs), calibrators, current amplifiers, and several peripheral devices is assembled and a local network to communicate with the instrumentation via Ethernet and IEEE-488 GPIB communication channels is setup. LabView is used to program the calibrators and amplifiers to output time-varying, noncyclic DC signals as virtual power using models to simulate real-world EV battery charging and measure their outputs through the DMMs. Virtual power is produced using two separate circuits—one providing voltages of 600-800 VDC and another providing currents of 100-200 A. The product of the voltage and current measurements integrated over time yield the virtual energy output. By comparing the value computed from the laboratory measurements to those registered on a DC power energy meter, a correction factor is generated and can be applied to the meter. Calibration programs are run on the various instrumentation to achieve a calibrated correction factor with errors on the order of 0.01 to 0.05 percent.

This service will ultimately provide a means for industry to calibrate DC power energy meters, which will in turn calibrate EVSE and charging stations used to directly charge EVs.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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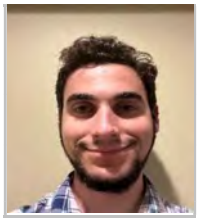
|---|---|
| **Name:** Andrew Peters | |
| **Academic Institution:** Florida State University | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | 1st Year Graduate Student |
| **Future Plans (School/Career):** | PhD in Physics |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Lab, Quantum Measurement Division, Fundamental Electrical Measurements Group |
| **NIST Research Advisor:** | Dr. Angela Hight Walker |
| **Title of Talk:** | The Missing Link: Automation of Magneto-Optical Spectroscopy of Quantum Materials |


**Abstract:**

Two-dimensional (2D) hybrid organic-inorganic perovskites have unique properties such as high coherent emission, spin-orbit coupling, and strong light-matter interactions, making them strong candidates for optoelectronic and spintronic applications. Magneto-Raman and magneto-photoluminescence (PL) spectroscopy are powerful techniques that allow one to study the symmetry and magnetic response of the quasiparticles (ex. phonons, magnons, excitons) in novel quantum materials such as 2D perovskites, graphene, carbon nanotubes, and transition metal dichalcogenides (TMDs). Our group's unique measurement capabilities allows for the quantitative control of the polarization of both the incident and scattered light, as well as the magnetic field and temperature. Experimentally, however, the quantitative control of the polarization within a magnetic field is not trivial. As light passes through an objective within a magnetic field, its polarization is rotated; a phenomenon called the Faraday effect. To have full control over the incident and scattered light, the Faraday effect must be accounted for at each magnetic field and temperature. In practice, this is done using two half-wave plates. One rotates the polarization of the incident light and the other rotates the polarization of the scattered light. When set correctly, the rotation caused by the Faraday effect is negated. This process was automated with a LabVIEW program. We calibrated the automated setup by performing polarized Raman spectroscopy on a Si/SiO2 substrate and a 2D perovskite, hexylammonium iodide. As a result, we determined the cut of the silicon substrate and the symmetry of the phonons from Raman signal and the symmetry of the exciton from PL.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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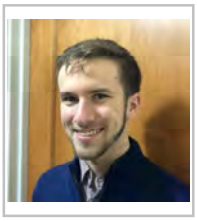
|---|---|---|
| **Name:** Brady Egleston | | |
| **Academic Institution:** University of Maryland-College Park | | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Junior | |
| **Future Plans (School/Career):** | To go to graduate school and become a physicist | |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory (PML) | |
| **NIST Research Advisor:** | Dr. Ian Spielman | |
| **Title of Talk:** | Characterizing $^{39}$K MOT clouds with Neural Networks | |

**Abstract:** With current methods, assessing the quality of the cloud of atoms in a magneto-optical trap (MOT) and determining its temperature and the number of atoms in the cloud are both processes that often require taking a time-of-flight absorption image. However, taking this image requires destroying the MOT, so one cannot gather these numbers and continue working on the same cloud. We are investigating ways of getting around this barrier by developing machine learning (ML) techniques combined with fitting 2D Gaussians and 2D Hermite-Gaussian models that would be applied to the cloud non-destructive fluorescence images to extract this information. Our goal is to train neural networks to estimate the characteristics of a MOT cloud described above. Moreover, by reducing the fluorescence images to a tabular format with a series of numbers not only significantly reduces the complexity of the ML models needed to process the data but also opens a path to invoking explainable ML to determine the importance of various fit parameters.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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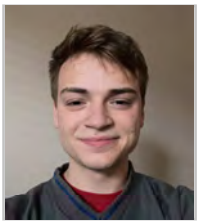
|---|---|---|
| **Name:** Noah Zuckman | | |
| **Academic Institution:** | University of Maryland, College Park | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Graduated | |
| **Future Plans (School/Career):** | Extending internship through next year, then starting a PhD in physics | |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Quantum Measurement Division, Atomic Spectroscopy Group | |
| **NIST Research Advisor:** | Dr. Joseph Tan | |
| **Title of Talk:** | Analysis of test data from the portable EBIT for NIST Boulder | |

**Abstract:**

A 0.7 Tesla electron beam ion trap has been designed and constructed in the Atomic Spectroscopy Group. It will be installed in the Boulder campus. Its extremely compact geometry utilizes radially polarized permanent magnets. We have begun observing X-ray spectra from highly ionized noble gases using a silicon drift detector (SDD). Electron Beam Ion Traps (EBITs) are used to create and trap highly charged ions (HCIs). Recent theoretical works indicate that certain HCIs can be used to test for variations in the fine structure constant over the lifetime of the universe and may serve as stable optical frequency standards. Moreover, well-known spectra from H-like and He-like ions can be used to evaluate novel quantum sensors, such as Transition-Edge Sensors (TES), providing SI-traceable calibration. Our objectives are to identify emission lines, calibrate the SDD X-ray detector, and prepare the mini-EBIT for installation in the Quantum Sensor Group in NIST Boulder. In early tests, X-ray emission lines observed by the SDD detector include He-like Ne and He-like Ar, though some strong lines remain unidentified. This mini-EBIT system is being ruggedized for transportation, and electro-pneumatic controls are being installed for vacuum management. The preliminary analysis provides valuable insights into the emission properties of highly ionized noble gases, serving as a foundation for future investigations, such as experiments using TES spectrometers with much higher resolution. This research contributes to the advancement of measurement science and facilitates the development of high-resolution X-ray spectrometers.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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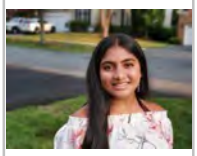
|---|---|
| **Name:** Joshua Young | |
| **Academic Institution:** University of Kentucky | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Pursue Graduate Degree in Nuclear Physics/Precision Measurement |
| **NIST Laboratory, Division, and Group:** | PML, Radiation Physics Division, Dosimetry Group |
| **NIST Research Advisor:** | Dr. Ronald Tosh |
| **Title of Talk:** | Development of an Ultrasonic Calorimeter for Dose Rate Imaging |


**Abstract:**

Radiotherapy for cancer treatment seeks to deliver radiation dose to tumors while sparing surrounding healthy tissue. Such selective delivery of dose has led to the development of various ingenious methods for spatially masking and directing beams to minimize exposure of healthy tissue while targeting tumor volumes. More recently, a dose rate effect has been discovered that indicates radiation sensitivity of healthy tissue decreases at sufficiently elevated dose rate, thus high dose rates in combination with spatially conformal irradiations (FLASH radiotherapy) are attracting much attention within the radiotherapy community.

This has presented a number of challenges for absolute dose metrology, which has been developed for use in spatially uniform dose fields at conventional dose rates. Accordingly, NIST has been working on an ultrasonic imaging technology to address difficulties posed by clinically relevant, spatially nonuniform fields, and part of the current project is dedicated to producing software simulations of radiation heating, ultrasonic data acquisition, and image processing to assist with design problems of that prototype instrument. Another aspect of the current project is to assess the suitability of ultrasound for imaging dose-rate fields by looking for spectral features attributable to dose-rate effects of interest to the radiotherapy community.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023


**Name:** Alisha Patel

**Academic Institution:** University of Maryland, Baltimore County | **Major:** Biochemistry and Molecular Biology

**Academic Standing (Sept. 2023):** Third-year Undergraduate

**Future Plans (School/Career):** Attend pharmacy school and possibly pursue a career in nuclear pharmacy

**NIST Laboratory, Division, and Group:** Physical Measurement Laboratory, Radiation Physics Division, Radioactivity Group

**NIST Research Advisor:** Brittany Broder, Denis Bergeron


**Title of Talk:** Analyzing the Effects of V-Vial Parameter Changes on Ionization Chamber Response Using TOPAS


**Abstract:**

Radiopharmaceuticals are useful agents in diagnosing and treating cancer. Measuring activity ensures the patient receives a sufficient amount of the treatment without it being harmful to the patient. A key tool to measuring administered activity accurately is the ionization chamber (IC). In an IC, radiation emitted from a source interacts with a fill gas, ionizing it. The electrodes within the IC create an electrical current from the ionized gas which is proportional to the activity of the source. IC response is sensitive to parameters such as the height of the source in the IC, the volume of the source solution, and dimensions of the source container. These effects cause different interactions with matter before reaching the fill gas and therefore, resulting in variations of IC response. Knowing the effects of these changes is important for measuring (and subsequently, administering) precise dosages. These effects are smaller for high-energy photon (gamma) emitters and are more pronounced for low-energy emitters. The majority of the IC response comes from photons, so low-energy emitters such as alpha and beta emitters are harder to measure. Yttrium-90 ($^{90}$Y) is a pure beta emitter with a half-life of 2.65 days and is currently used to treat liver cancer. The short range and high energy deposition of beta particles makes $^{90}$Y an excellent therapeutic agent as most of its induced damage targets the tumor. However, there are challenges when modeling and measuring the administered activity because no photons are emitted directly from $^{90}$Y decay and thus, the instrument response arises mostly from bremsstrahlung interactions. Like many pharmaceuticals, a $^{90}$Y dose is typically prepared in a v-vial. In this project, the Geant4-based Monte Carlo program TOPAS is used to model the Vinten 671 ionization chamber (VIC) and assess the effects of various vial parameters on IC response. TOPAS is a useful tool in exploring the impact of geometry parameters as it allows several possibilities to be modeled and the impact on IC response to be observed. The results can then be compared to historical data. New source geometries were modeled, and the sensitivity of the VIC response was investigated.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Ethan Zheng | |
| **Academic Institution:** University of Southern California | **Major:** Physics and Computer Science |
| **Academic Standing (Sept. 2023):** | Sophomore |
| **Future Plans (School/Career):** | PhD in nuclear or quantum physics, become research scientist or professor. |
| **NIST Laboratory, Division, and Group:** | PML Radiation Dosimetry Group |
| **NIST Research Advisor:** | Csilla Szabo-Foster |
| **Title of Talk:** | The modelling and testing of the Wide Angle Free Air Chamber |

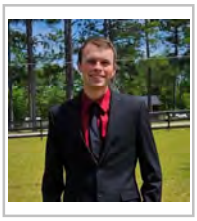

**Abstract:**

The area of study pertains to the dosimetry group, specifically the measurement of radiation emitted by radioactive seeds used in brachytherapy. Dosimetry is the process of relating the administered amount of radioactivity to the absorbed radiation dose in tumors, organs, or the whole body. The dosimetry group at NIST is primarily focused on finding acceptable amounts of radiation for radioactive seeds that are used to treat cancerous tumors in the body.

Radiation has been used to treat tumors since Marie Curie's research and discoveries in radioactivity and its properties. The dose of radiation in a brachytherapy seed should be enough to destroy the tumorous cells but not affect the living tissue surrounding it. The measurement for this radiation is called air-kerma, kerma being the kinetic energy released per unit mass of a small volume of a medium by ionizing radiation (J/kg).

The research is focused on the modeling of the machine that measures the amount of air-kerma in a radioactive seed, known as the Wide Angle Free Air Chamber (WAFAC). Using a strong electric field, the WAFAC is able to measure the radioactive ways emitted by a seed. Modeling this machine in a physics simulation program COMSOL will allow us to better understand what the electric field lines in the machine look like and also how external disturbances might affect the field lines and therefore the measurement of air-kerma.

The long term goal is to have a working model of the WAFAC machine in COMSOL that will allow researchers to study the electric field lines generated by the machine under different circumstances which will allow for a better understanding of how the WAFAC operates without the need to have the machine present or running.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Travis White Jr. | |
| **Academic Institution:** Mercer University | **Major:** Mechanical Engineering |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Attending graduate school and conducting engineering in aerospace |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Office of Weights and Measures, Laboratory Metrology |
| **NIST Research Advisor:** | Isabel Baucom |
| **Title of Talk:** | Analyses in Laboratory Metrology |

**Abstract:**

Metrology, the science of measurement and measurement applications, remains essential in science and commerce. NIST's Laboratory Metrology Program aims to ensure traceability of weights and measures calibration standards to the International System of Units. This program accomplishes its mission by providing training, developing documentary standards, extending laboratory recognition, and testing laboratory proficiency for both state laboratories and private laboratories. Throughout the SURF Program, software utilized in the Fundamentals of Metrology training course was verified and validated to ensure accurate and proper function. Moreover, data sets from this course were analyzed to determine metrologist proficiency, process control, and artifact stability. Further measurements were collected and examined to affirm this data. Internal auditing was conducted according to ISO 17043 Conformity Assessment to validate the proficiency program's compliance to international laboratory standards. Additionally, historical proficiency testing data was evaluated to determine the stability of artifact measurement results over time. This data analysis initially focused on Mass Echelon class artifacts. According to the State Laboratory Program Workload Survey, 44 reporting laboratories performed approximately 260,000 mass calibrations for legal metrology and United States industry in 2020. These services are crucial to ensure the validity of the measurement system and measurement calibrations performed throughout the national economy. These reviews and evaluations for the Laboratory Metrology Program have improved and validated procedures and documents to ensure stable calibration methods and traceable measurement services in laboratory metrology.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

**Name: Dinelka Jagoda**

| **Academic Institution: University of Maryland, College Park** | **Major: Computer Science** |
|---|---|

**Academic Standing (Sept. 2023): Academic Honors**

**Future Plans (School/Career): Earn B.S degree in Computer Science from UMD**

**NIST Laboratory, Division, and Group: Office of Weights and Measures (OWM), Metric Program**

**NIST Research Advisor: Ms. Elizabeth Benham**

**Title of Talk: OWM Educational Outreach Resources**

**Abstract:** The NIST Metric Program publishes a variety of K-12 educational materials and curates an extensive website to help classroom educators facilitate student application of International System of Units (SI) skills. Resources include hands-on activities, videos, guides, and homework helpers that enrich classroom curriculum and reinforce student learning. Being an intern for this program has provided me with valuable insights into the significance of the SI in both academic and everyday contexts. Through my involvement in enhancing and developing educational resources related to the SI, I have been able to pursue my passion for assisting fellow students and engage in formal design work. As part of my responsibilities, I have gained experience in reviewing publications, evaluating web pages, and creating interactive SI activities. For instance, I have published a multi-set card game aimed to help students learn about the SI defining constants, base units, derived units with special names, and the prefixes. Furthermore, to prepare for the upcoming 2024 Olympic games, which is a significant opportunity for the U.S. general public to increase familiarity with a variety of SI measurements, I have implemented additional enhanced information and content for the “Metric and Sport” website. In addition to my primary projects, I have been involved in other significant tasks such as creating an informative poster about the OWM office for the 2023 NCSL International Workshop & Symposium. Furthermore, to fulfill a significant gap in website content, I collaborated with another intern to research, curate, and implement a new “SI derived units with special names” education webpage. Lastly, to expand NIST resources for upper elementary school audiences, I applied my graphic design skills to research and help produce a “How to use a metric ruler” video.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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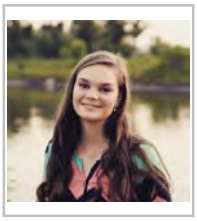
|---|---|
| **Name:** | Jeremy Robin |
| **Academic Institution:** | Washington University in St.Louis |
| **Major:** | Physics/Computer Science |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Not sure |
| **NIST Laboratory, Division, and Group:** | PML, Division 681, Group 05 |
| **NIST Research Advisor:** | Arvind Balijepalli |
| **Title of Talk:** | Multiplexed Electrochemical Biosensing |


**Abstract:**

Electrochemical biosensors are useful for measuring biological activity, such as DNA hybridization or enzyme activity or pH measurements. These electrochemical devices have become extremely powerful and are able to sense microscopic biological process. Now electrochemical biosensors have become an essential part of personalized medical care. For example, they can be used to detect certain enzymes in the blood like a glucose sensor for a diabetes patient or enzymes that may be an indicator for Alzheimer's disease. Diagnosing medical problems will be cheaper and more cost effective the more that these devices can be miniaturized and used simultaneously.

A critical advantage of electrochemical sensors is the possibility of developing highly parallel chip-scale measurements that can simultaneously detect multiple analytes. My goal this summer is to enable such a multiplexed measurement system to automate operation. For this I developed LabVIEW code to multiplex the sensors, control ancillary instrumentation such as pressure pumps that transport analyte solutions onto the biosensors and perform data analysis. I tested the system initially with pH measurements and plan to perform DNA hybridization measurements. In addition to purely medical benefits, this form of automated and paralleled measurements serves to remove error from an experiment and increase repeatability of the experiment.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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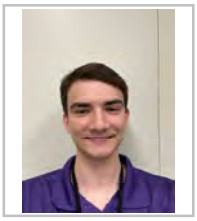
|---|---|
| **Name:** | Ginny McCracken |
| **Academic Institution:** | Shorter University |
| **Major:** | Biochemistry |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Forensic toxicology |
| **NIST Laboratory, Division, and Group:** | PML, Microsystems and Nanotechnology division, 681.05, Biohpysical and Biomedical Measurement Group |
| **NIST Research Advisor:** | Darwin Reyes-Hernandez |
| **Title of Talk:** | Fabrication and Characterization of Functionalized Graphene Field Effect Transistor for the Quantification of Exosomes Produced by Induced Pluripotent Stem Cell-Derived Cardiomyocytes |

**Abstract:**

Cells release extracellular vesicles (e.g., exosomes) that are primarily responsible for intercellular communication and the exchanging of biological material in physiological and disease conditions. Recently, it has been shown that exosomes can play a key role in regeneration of heart tissue after myocardial infarction. A fabricated heart-on-a-chip (HoC), comprised of human induced pluripotent stem cell-derived cardiomyocytes, will be used to release exosomes under physiological and pathophysiological conditions. To quantify exosome levels, we will use a graphene field effect transistor (gFET) functionalized with specialized antibodies. The gFET will be made from commercially available graphene transferred to a Si/SiO2 substrate wafer using PMMA-assisted wet transfer, with electrodes made using a lithography/lift-off process. The attachment of an exosome to an antibody in the channel of a gFET creates a change in the charge carrier density in graphene, leading to an alteration in the current and subsequently the impedance. Imminent experiments will determine the optimal antibody concentration for the gFET, which will inform the assembly of the sensor for further testing. The fabricated gFET can potentially be paired with other biological systems to produce real-time monitoring of the progression of cells.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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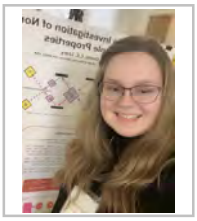
|---|---|
| **Name:** Connor Skelton | |
| **Academic Institution:** Milwaukee School of Engineering | **Major:** Biomoleculer Engineering |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Graduate with Bachelors and go into Industry |
| **NIST Laboratory, Division, and Group:** | PML, Div 681, Flow Cytometry |
| **NIST Research Advisor:** | Gregory Cooksey |
| **Title of Talk:** | Uncertainty Quantification in Flow Cytometry with AM Modulation |


**Abstract:**

The focus of our research is to provide precise uncertainty quantification to measurements in flow cytometry, a field that uses instruments to study cells as well as micro- and nanoparticles. This research will help develop and advance the precision of particle measurements in the biomanufacturing, drug discovery, and biotechnology industries. Using NIST-developed flow cytometers that can measure each particle multiple times, we can determine the measurement uncertainty associated with each particle's optical properties. These uncertainty measurements separate the measurement uncertainty from the inherent population distribution, thus enabling better classification of particles. The use of multiple measurement regions implies a benefit in reducing the number of required detectors, so we have started developing a method to encode each region with a unique laser modulation frequency (i.e., amplitude modulation (AM)), such that all signals can be collected on a single detector and separated using a demodulation algorithm. In order to understand the limits of AM cytometry, we have embarked on a study of how various components of the AM process impact affect the uncertainty of the signals of interest.

We have developed MATLAB algorithms to simulate the effects of noise on particle data to see the direct effect on the uncertainty quantification of collected data points. We simulated a measurement process by passing particles through an image of the laser profile and modulating the output waveform, and will study various noise characteristics we have measured in a cytometer. Particle abnormalities such as crosstalk between interrogation regions, particle overlaps, and demodulation scaling can also be simulated and interpreted. We will use this data to project how using AM impacts the dynamic range and uncertainties associated with measurements. For validation, we have also begun collecting data using fluorescent microparticles with and without amplitude modulation.

Ultimately, this analysis will enable techniques that utilize more measurement regions for the purpose of



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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| **Name:** Olivia Green | | |
| **Academic Institution:** | The College of Wooster | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Senior | |
| **Future Plans (School/Career):** | I will be attending Case Western Reserve University in the fall to pursue my PhD in physics. | |
| **NIST Laboratory, Division, and Group:** | PML, Sensor Science Division (685), Thermodynamic Metrology group (01) | |
| **NIST Research Advisor:** | Daniel Barker | |
| **Title of Talk:** | Testing the performance of optomechanical pressure sensors | |


**Abstract:**

We present tests of the pressure-sensing performance of optomechanical membranes and trampolines. In these optomechanical devices, the pressure is evaluated from the background-gas-induced mechanical damping rate using the kinetic theory of gases. We measure the damping rate for helium, nitrogen, and argon partial pressures from 0.1 mPa to 1000 Pa using a Michelson interferometer. We find that mechanical ringdown measurements of the damping rate are more reliable in the medium vacuum range (0.1 Pa to 100 Pa) and below, while thermomechanical noise measurements perform better in the low vacuum range (above 100 Pa). We compare the pressure inferred using both damping rate measurement methods to the pressure measured by a calibrated capacitance diaphragm gauge suite. Intrinsic thermal damping from the substrate currently limits the linear operation range of our devices to the medium vacuum. We discuss prospects for reducing the intrinsic damping rate and fiberizing the Michelson interferometer to realize optomechanical pressure sensors beyond the lab.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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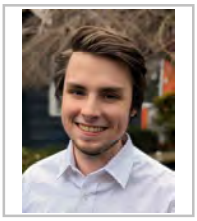
| **Name:** | Benjamin Baldwin |
| **Academic Institution:** | University of Maryland |
| **Major:** | Chemistry |
| **Academic Standing (Sept. 2023):** | Graduated |
| **Future Plans (School/Career):** | Ph.D. in Physical Chemistry |
| **NIST Laboratory, Division, and Group:** | PML, Sensor Science Division, Thermodynamic Metrology Group |
| **NIST Research Advisor:** | Eric B. Norrgard |
| **Title of Talk:** | Rotational Cooling of a Molecular Beam |


**Abstract:**

Ultracold molecules are central to quantum information science, precision metrology and fundamental physics research. To reach temperatures below 1 mK, typical atomic and molecular cooling and trapping setups use a combination of Doppler cooling and magneto-optical traps in which laser radiation facilitates the repeated excitation and relaxation of molecules or atoms in a process called photon cycling.

When compared to atoms, the additional rotational and vibrational degrees of freedom in molecules often complicate cooling and trapping schemes. Target molecules can escape the the cooling cycle through decay after excitation to different rotational states not addressed by the main cooling lasers. We can eliminate some of these decay pathways by driving the transition from N=1 in the ground state to N=0 in the excited state, where N describes the molecule's rotational energy level. Selection rules in quantum mechanics disallow certain decays involving rotational states, so this transition proves favorable in efficient optical cycling, but not all molecules reside at N=1. At the outset of cooling and trapping setups magnesium monofluoride (MgF) travels in a cryogenic buffer gas beam (CBGB) at a temperature of ~4K, where there is still a significant population of molecules in higher-energy rotational states N>1.

We use microwave frequencies to drive magnesium monofluoride (MgF) molecules from N=2 to N=3, and optical frequencies to drive from N=3 to N=1. Rotational cooling success is gauged by an increased population of MgF in the N=1 state, as these molecules can then be cooled by the main photon cycling frequency. We use laser-induced fluorescence to measure the number of molecules in N=1 and compare to baseline population without rotational cooling in the CBGB.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Gabriel Kuntz |
| **Academic Institution:** | Seattle University |
| **Major:** | Physics & Computer Science |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Attend Graduate School studying Quantum Computing/Related Field or Flight School |
| **NIST Laboratory, Division, and Group:** | PML 685-01, Sensor Science Division, Thermodynamic Metrology |
| **NIST Research Advisor:** | Stephen Eckel |
| **Title of Talk:** | Developing a robust and cost-effective digital PID controller for laser cooling |


**Abstract:**

Laser cooling and trapping of atoms requires precise control of the trapping laser intensity and frequency. In the cold atom vacuum standard (CAVS), used to measure pressure at ultra-high and extreme-high vacuum ranges, laser intensity noise causes inaccurate counting of atoms that leads to uncertainty in the pressure measurement. In order to adapt to small changes in the system, a proportional-integral-derivative (PID) controller is used to feedback on a photodiode signal to produce a steady and controlled laser intensity. However, off-the-shelf analog and digital PID controllers often lack features, like integrator blanking or holding, which limits their usefulness for laser intensity stabilization. We present a robust PID controller based on the Moku family of reconfigurable hardware platforms, which use field programmable gate arrays (FPGAs) for onboard computation. FPGAs allow for the creation and modification of digital circuits to perform digital signal processing. The Moku devices have a user-friendly, web-based integrated development environment (IDE) that allows customization of the onboard FPGA. Using the Moku, we built a PID with integrator blanking and holding to counter the effects of integrator wind-up and remove laser turn-on delays in experiment. To demonstrate the efficacy of the PID controller, we measured its locking bandwidth and tested it on the experimental apparatus.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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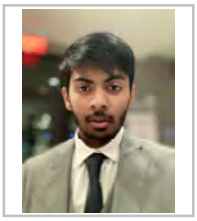
| **Name:** Grace E. Waters | |
| **Academic Institution:** Virginia Military Institute | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Graduate (with B.S. in Physics with distinction (minor) in Astronomy and Applied Mathematics) |
| **Future Plans (School/Career):** | Explore opportunities that center my career around the STEM field and possibly obtain a graduate degree at some point in the future |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Sensor Science Division, Surface and Metrology Group |
| **NIST Research Advisor:** | Dr. Aaron Goldfain |
| **Title of Talk:** | Measuring the Bidirectional Reflectance of Materials for UVC Germicidal Applications |


**Abstract:**

UV radiation is an effective way to disinfect public spaces. Traditional UV disinfection systems emit radiation at wavelengths that range from 255 nm to 280 nm. However, newly designed systems are being manufactured to emit UV radiation at 222 nm. At 222 nm specifically, the radiation is mostly absorbed by the layering of dead skin cells on the human body. Additionally, the proteins on top of the human eye also absorb the 222 nm radiation, causing little harm to any part of the eye. Thus, it is significantly less harmful than 255 nm to 280 nm radiation and is potentially more effective at killing pathogens. In order to successfully determine the radiation dose delivered to surfaces and room occupants, manufacturers need information on the directional reflectance of common building materials within the spectral range of 222 nm to 280 nm, which has not been fully determined thus far. The goal for my project is to contribute to an open access directional reflectance database towards improving UV disinfection technology by enhancing its efficiency and safety for disinfecting public spaces.

This project involves measuring the bidirectional reflectance of materials within the UVC spectral range using a commercial spectrophotometer with a directional reflectance accessory. This accessory measures light reflected off the sample from an under-illumination source from the main spectrophotometer. The samples are measured at different wavelengths: 280 nm, 255 nm, and 222 nm. The measurements are typically repeated at different sample orientations: 0, 90, and 180 degrees clockwise. The resulting data is processed to calculate the Bidirectional Reflectance Distribution Function, BRDF, and plotted with uncertainties corresponding with each wavelength. Currently, the measurements and plots present interesting variation throughout each sample measured in different orientations and angles. Any change in the angle of detection, the angle of the sample, and its orientation impact the BRDF of the material.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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| **Name:** | Rishabh Sinha |
| **Academic Institution:** | University of Maryland -- College Park |
| **Major:** | Computer Science |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Masters or PhD in Computer Science |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Sensor Science Division (685), Remote Sensing Group (04) |
| **NIST Research Advisor:** | Solomon Woods |
| **Title of Talk:** | Simulation and Measurement of 3D Thermal Gradients in Liquids for Magnetic Imaging Validation |


**Abstract:**

3D thermal imaging based on Magnetic Particle Imaging (MPI) has the potential to provide an unprecedented non-invasive approach to accurately monitor temperature variations in the human body, thereby revolutionizing disease detection protocols and therapy response evaluation in the medical sector. Our research investigates the use of MPI to quantify temperature by measuring signal harmonics of magnetic nanoparticles subjected to alternating magnetic fields. This novel approach to sensitive and accurate 3D Thermal Imaging can observe temperature variations in relation to magnetic signals in each voxel, establishing a dependence between magnetic response and temperature. At this juncture, we need to validate our magnetic imaging results by comparison with simulations of non-uniform thermal fields.

The simulations employ a custom Finite Element Analysis (FEA) model to simulate miniature quartz cubes with nanoparticle fluid wells (thermal phantoms) and material systems that are experimentally imaged to visualize temperature gradients in 3D. Through the use of COMSOL Multiphysics we have established a framework for 3D thermal imaging simulations based on measurements of magnetic nanoparticle tracers in thermal phantom samples and other particle heating experiments. Simulation results were plotted through Matplotlib and Matlab. Additionally, signal generation is being enhanced through parallel processing for 2D phantoms. Our research utilized a FEA solver to simulate time-dependent, convective heat-flux, and equilibrium states, effectively determining a 3D temperature map from data about defined heat sources, isotherms, material properties, and boundary conditions.

Our findings provide 2D and 3D thermal gradient data for direct comparison with temperature-dependent MPI using multi-harmonic detection, as well as magnetic nanoparticles with oscillating fields. We also observed a spatial resolution dependence on harmonic number when temperature is considered, which carries significant implication for image reconstruction.

# SURF Student Colloquium

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August 1-3, 2023

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| **Name:** Dawn Pierce | |
| **Academic Institution:** George Mason University | **Major:** Astronomy |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Exoplanet Research |
| **NIST Laboratory, Division, and Group:** | PML, Sensor Science Division, Remote Sensing Group |
| **NIST Research Advisor:** | Susana Deustua, Thinh Bui |
| **Title of Talk:** | Measuring the UV Transmittance of DMDs and How It Will Help Us Search for Habitable Exoplanets |


**Abstract:**

Currently, the most accurate standard star flux calibrations have an uncertainty of 1%. Bringing this uncertainty down would allow us to measure stellar parameters more precisely and subsequently improve our ability to characterize exoplanets. Knowledge of a star's variability at ultraviolet wavelengths is especially useful to astronomers and astrobiologists since a star's activity in the ultraviolet band can influence the habitability of the exoplanets around it. The challenge of reducing this percentage is being tackled with CANDLE (Calibration using an Artificial star with NIST-traceable Distribution of Luminous Energy), a prototype satellite payload of calibrated light sources being developed at NIST with NASA funding. One of these illumination modes, the programmable spectrum (PS) projector, utilizes a digital micromirror device (DMD) to reflect dispersed light at certain frequencies at specific intensities. Due to the properties of the DMD, however, it acts as a blazed grating and loses light due to diffraction. DMD diffraction has been measured for light in the visible and near-infrared wavelengths, but no studies have been done for how much light is lost in the ultraviolet and infrared bands. In order to properly calibrate a DMD for use in the PS mode, more knowledge was needed regarding its reflective and diffractive properties when exposed to ultraviolet light. To test these properties, lenses were first set up on an optical bench to feed light from an ultraviolet light source into an integrating sphere using optical fibers. The light was then sent to a spectrometer such that the spectrum could be measured and compared with a known standard. With the transmittance of the optical fibers understood, the next steps are to add a DMD into the array of lenses to measure the light lost due to diffraction and to measure how reliably DMDs can reflect a given spectrum over time.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** Briana Chen | |
| **Academic Institution:** Purdue University | **Major:** Aerospace Engineering/Applied Physics |
| **Academic Standing (Sept. 2023):** | Junior |
| **Future Plans (School/Career):** | Graduate school! |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Sensor Science Division, Remote Sensing Group |
| **NIST Research Advisor:** | Thinh Bui, Susana Deustua |
| **Title of Talk:** | Measuring digital micromirror device characteristics in the infrared wavelength regime |

**Abstract:**

In cosmology, accurate flux measurements can improve the precision of constants related to the accelerated expansion of the universe, possibly even resolving contradictions such as Hubble's tension. This requires minimization of flux uncertainties: instruments like the James Webb Space Telescope, Roman Space Telescope and Rubin Observatory must control these uncertainties through precise calibration standards. Currently, researchers at NIST are developing an artificial stellar source called CANDLE (Calibration using an Artificial star with NIST-traceable Distribution of Luminous Energy) which will improve calibration of ground and space-based telescopes by sending stable light with calibrated flux, wavelength, and beam profile. Within CANDLE, the Programmable Spectrum Mode (PS) simulates astronomical sources by shaping solar flux of wavelength range 310-2500 nm to the desired spectra, which is then beamed towards telescopes to calibrate accordingly. This wide spectrum requires different optical setups, leading the CANDLE team to split the PS mode into 4 spectral bands. A digital micromirror device (DMD) is used to "select" wavelengths and their corresponding intensity for the spectra and must be characterized for each wavelength band: specifically, reflection and transmission of light off the DMD occur differently based on the wavelength. This project studies the characteristics of the SWIR (short wave infrared region) DMD by measuring the reflectance and transmittance of the DMD for the SWIR wavelength band. This is important as these properties will tell us how much light is needed to input into the system to account for losses. Furthermore, DMDs can be modeled by a blazed diffraction grating and different pitches of a DMD will change the properties of diffraction such as the blaze wavelength. Because diffraction by the DMD becomes prominent at longer wavelengths, consequently reducing the amount of usable light coming from the DMD and affecting the spectra, measuring the DMD diffraction efficiency along with the existing transmittance and reflectance properties will help simulation of the PS mode optics, ultimately extending the capabilities of CANDLE into SWIR.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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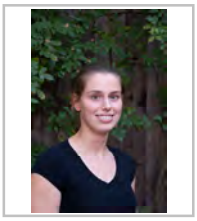
| **Name:** Colleen Ewald | | |
| **Academic Institution:** | University of Colorado Boulder | **Major:** Astronomy and Mathematics |
| **Academic Standing (Sept. 2023):** | Sophmore | |
| **Future Plans (School/Career):** | Unsure | |
| **NIST Laboratory, Division, and Group:** | Physical Measurements Laboratory, Sensor Science Division, Remote Sensing Group | |
| **NIST Research Advisor:** | Joe Rice | |
| **Title of Talk:** | Impact of the Degradation rate of Photodiodes on CANDLE Project | |


**Abstract:**

For the past 50 years, astronomers have been using data traceable to a single standard star (Vega) to calibrate their telescopes and observatories. However, recent data suggests that this star might not be the best standard candle due to fluctuations in its light and other issues. There are several ways to solve this problem of inaccurate calibrations. One way is the Calibration using an Artificial star having NIST-traceable Distribution of Luminous Energy (CANDLE) project led by NIST. This project proposes to launch a satellite to space with the purpose of being used as a standard candle star. When CANDLE is launched to space, its light sources on board the satellite must be calibrated for spectral irradiance and have a known uncertainty, otherwise it is no better than what we currently have. The challenge presented is that instruments such as light sources and sensors generally degrade faster in the harsh environment of space. As such we must assess the degradation of instruments in space so that we can be confident in our uncertainty. A photodiode is one such instrument that we must assess its degradation in space. Photodiodes are used to determine the solar irradiance from the Sun. This is important because the light source that CANDLE will use and send down to the observatories on Earth is the Sun. The Laboratory for Atmospheric and Space Physics (LASP) at the University of Colorado, Boulder, has had for the past five years a scientific device called the Total and Spectral Solar Irradiance Sensor (TSIS - 1) attached to the International Space Station (ISS). The TSIS has three channels that measure the Sun's solar spectral irradiance using both photodiodes and Electrical Substitution Radiometers (ESRs) at different time intervals. We can as such use their data to assess the degradation of the photodiodes. The results from this analysis will impact which photodiodes are installed on the CANDLE project.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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| **Name:** Amanda Younes | |
| **Academic Institution:** University of California, Los Angeles | **Major:** Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | PhD in Physics |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, Sensor Science Division, Thermodynamic Metrology Group |
| **NIST Research Advisor:** | David La Mantia |
| **Title of Talk:** | Rydberg atom sensing of blackbody radiation |


**Abstract:**

Objects at finite temperature emit energy in the form of blackbody radiation (BBR), which is incoherent electromagnetic radiation with a continuous frequency spectrum whose peak corresponds to the body's temperature. Rydberg atoms, or atoms with a highly-excited valence electron, can be used as sensors of BBR due to their large electric dipole moments which make them very sensitive to electric fields, as well as the primary, calibration-free nature of atomic systems. Given a good BBR sensor, one can characterize the temperature of the blackbody that emitted the radiation.

To measure temperature using BBR, we consider the population dynamics of rubidium atoms in a vapor cell when excited to high-lying states. BBR can cause direct ionization, which can be easily detected by collecting the resulting ions. Additionally, BBR induces population redistribution among Rydberg states, which can be resolved using selective field ionization (SFI) by ramping an electric field to ionize different states at different electric field strengths. These measurements are used to deduce the nature of the radiation experienced by the atoms, and therefore the temperature of the BBR emitter. This data is collected at various atomic densities across many principal and orbital angular momentum quantum numbers in order to experimentally map out the behavior of atoms in the cell with external BBR and determine the method's viability as a temperature sensor.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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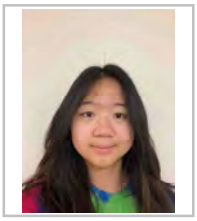
|---|---|
| **Name:** | Addhyaya Sharma |
| **Academic Institution:** | The City College of New York (CUNY) |
| **Major:** | Physics |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | Graduate school into industry |
| **NIST Laboratory, Division, and Group:** | PML, Division 681, Biophysical and Biomedical Measurement Group |
| **NIST Research Advisor:** | Dr. Joseph W. Robertson |
| **Title of Talk:** | Assembling DNA origami fused plasmonic nanopores for single molecule detection |


**Abstract:**

Plasmonic nanopores have emerged as a promising avenue for sequencing and single molecule detection, owing to their sensitivity to surface properties of the nanostructure and the dielectric properties of the environment. In this study, we create a single-nanopore sensor by inserting a protein cytolytic pore forming toxin into a lipid bilayer membrane that separates two electrolyte chambers. Ionic current flowing through the pore is measured with an applied electric field. When molecules of interest (e.g., DNA, proteins) partition into the pore, the ionic current is interrupted in a resistive pulse which can be inspected to provide details of the size and chemistry of the molecule. We are enhancing this sensor by constructing a DNA-nanotechnology scaffold to attach plasmonic gold nanoparticles to the sensor surface with nanometer-precision. These particles absorb light in their plasmon modes and rapidly thermalize the energy creating yoctoliter heat sources around the nanopore sensor. To predict the temperature distribution within the structure, we employ COMSOL simulations to investigate the 3D temperature gradient resulting from laser-induced heating of gold nanoparticles. We also explore the effects of various parameters such as the number, position, and size of the gold nanoparticles, as well as the laser power, on the resulting temperature distribution. Moreover, we determine the rise time and cooling time for the assembled structure. Concurrently, we conduct experiments related to the kinetics of assembly with the help of Surface Plasmon Resonance (SPR) and electrochemistry techniques. The objective of the study is to synthesize the insights obtained from simulations and bulk measurements to design a single molecule heating experiment that contributes to the advancement of sequencing and detection applications.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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| **Name:** Ziran Du | | | |
| **Academic Institution:** | Stony Brook University | **Major:** | Mechanical Engineering, Applied Math |
| **Academic Standing (Sept. 2022):** | Freshman | | |
| **Future Plans (School/Career):** | Graduate School | | |
| **NIST Laboratory, Division, and Group:** | PML | | |
| **NIST Research Advisor:** | Zachary Levine | | |
| **Title of Talk:** | Saturation of Susceptibility in a Two-Level System, a Model of a Rb Vapor Cell | | |

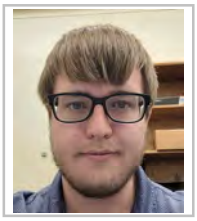

**Abstract:**

When a laser hits an atom, a valence electron interacts with its electric field by gaining energy and going to an excited state. The same electric field can also cause an excited-state electrons to return to the ground state. Excited state electrons can also fall to the ground state. These processes are called absorption, stimulated emission, and spontaneous emission.

We can study these behaviors by isolating cases. If there is no electric field, we see an exponential decay of the excited state electron. If we do not allow spontaneous emission, the population of the states oscillates periodically from ground to excited state at a frequency known as the Rabi frequency. A third factor which influences the changing states is the detuning of the electric field, where its frequency is not perfectly at the atomic resonance but slightly over of under, leading to an increase in the Rabi frequency.

The incoming electric field also produces an induced electric field from the atom. This is because the atom has some polariazability as well as the saturation constant which determines the nonlinear susceptibility. The saturation is how closely the ratio of the population of ground state to the excited state is 2:1, at which point the spontaneous emission rate equals the stimulated emission rate. When we graph the susceptibility vs the input E field, we see that the curve is approaching two asymptotic values, one is zero and the other is the linear susceptibility constant. The point of studying the two-level system in detail is to verify an the computer code which predicts susceptibility more generally.

Saturation of the susceptibility has been observed experimentally in a Rb vapor cells. We hope to extend our results to match experimental data by the time of the talk.



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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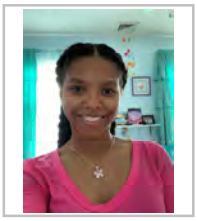
| **Name:** John Taylor | | | |
| **Academic Institution:** | Colorado School of Mines | **Major:** | Engineering Physics |
| **Academic Standing (Sept. 2023):** | Senior | | |
| **Future Plans (School/Career):** | Graduate School | | |
| **NIST Laboratory, Division, and Group:** | PML, Quantum Measurement Division, Applied Electrical Metrology Group | | |
| **NIST Research Advisor:** | Jason Underwood | | |
| **Title of Talk:** | Examining the Experimental Limitations of the Quantum Ampere | | |

**Abstract:**



# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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| **Name:** | Mya Merritt |
| **Academic Institution:** | Morgan State University |
| **Major:** | Engineering Physics |
| **Academic Standing (Sept. 2023):** | May. 2024 |
| **Future Plans (School/Career):** | Physicist |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory (PML), Quantum Measurement Division 684, Quantum Optics Group 03 |
| **NIST Research Advisor:** | Dr. Sergey Polyakov |
| **Title of Talk:** | Obtaining Super Resolution with Thermal States using Photon Number Resolving Camera |

**Abstract:**

While optical microscopy is a powerful tool in biology and medicine, all optical systems suffer from the Raleigh limit that limits the resolution of this measurement modality. To exceed an instrument's diffraction limit and obtain super resolution, an extra parameter must be employed. Here we study how photon counting, the direct consequence of the quantum nature of light can be used to obtain such an extra parameter. In our optical setup, quantized photons are acquired from a pseudo thermal state and detected with a photon number resolving camera. Never has a camera been used to obtain super resolution images with such thermal states. However, it is very practical as it efficiently collects data in a short amount of time, and it allows images to be taken with photon number statistics for each of its pixels individually. To use this camera reliably and verify its ability to count photons, we collect and statistically analyze the digital output of the camera. Particularly, we will establish the correspondence between the camera output and the true photon number.

# SURF Student Colloquium

NIST – Gaithersburg, MD

August 1-3, 2023

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|---|---|
| **Name:** | Justin Michael Craven |
| **Academic Institution:** | California State University Chico |
| **Major:** | Physics, Electrical Engineering |
| **Academic Standing (Sept. 2023):** | Senior |
| **Future Plans (School/Career):** | I plan to pursue a Ph. D. in Physics to preform research and teach at the university level. |
| **NIST Laboratory, Division, and Group:** | Physical Measurement Laboratory, 684, Rb/K Ultra-cold Atom Group. |
| **NIST Research Advisor:** | Dr. Ian Spielman |
| **Title of Talk:** | Faster ultracold atom data collection through the use of a one-dimensional optical molasses |

**Abstract:**

Ultracold experiments require a new population of trapped and cooled atoms for each experimental shot. In these apparatuses, hot atoms originate from a source and then travel through multiple cooling and trapping stages. Before these cooling and trapping stages the atoms form an atomic beam, the size of which plays an important role in the load time for each experimental shot. A more collimated atomic beam will result in a greater number of atoms reaching the magneto-optical trap (MOT), thus shortening the load time between shots. Our project is to implement a transverse one-dimensional optical molasses for a Rubidium 87 atomic beam. This was designed with the goal of further controlled collimation of the atomic beam resulting in faster data collection. The optical molasses consists of a detuned elliptical shaped 780nm diode laser which is counter propagated along an axis orthogonal to the desired atom path. The laser used is amplified by a tapered amplifier (TA) and frequency shifted or detuned with the use of an acousto-optical modulator (AOM) to produce an optimal cooling effect when used in conjunction with the Doppler effect. In utilizing the Doppler effect and a frequency detune we select which velocities result in a high or low chance of absorption and subsequent slowing. This prevents us from re-accelerating slow atoms or further accelerating hot atoms. Through a series of optics, the laser diode beam is expanded, polarized, and shaped to match the atomic beam dimensions and slow a wide sample of the distribution of atoms in the transverse axis. A simple retroreflector and waveplate reflects the laser light to constrict the distribution of atoms in the opposite direction simultaneously. We hope for a significant decrease in the loading times for each shot.