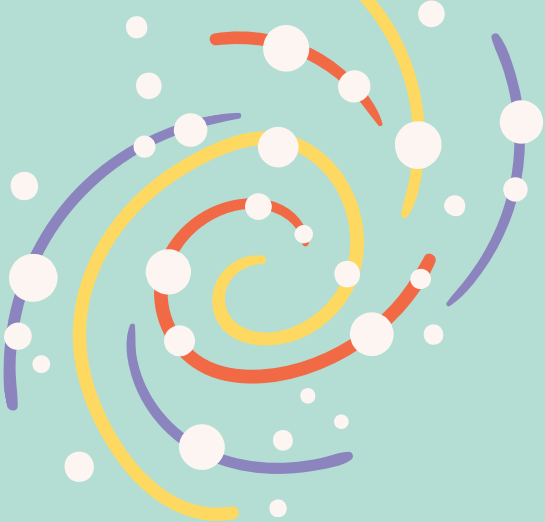
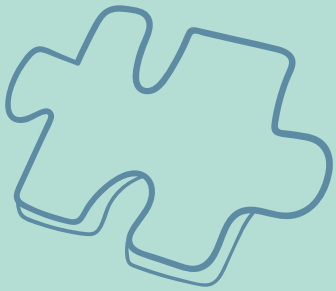
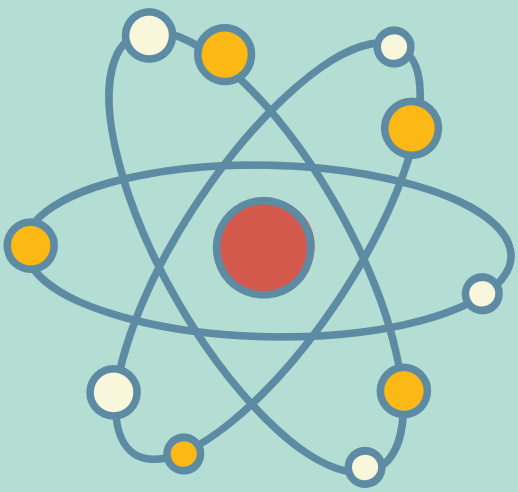




NIST | SUMMER UNDERGRADUATE RESEARCH FELLOWSHP

SURF 2022



Greetings,

On behalf of the Director's Office, it is my pleasure to welcome you to the 2022 SURF Colloquium. For the second year in a row, colloquiums are 100% virtual.

Founded by scientist in the Physics Laboratory (PL) with a passion for STEM outreach, the SURF Program has grown immensely since its establishment in 1993. The first cohort of the SURF Program consisted of 20 participants from 8 universities primarily conducting hands-on research in the physics lab. Representing all STEM disciplines, this summer's cohort of the SURF Program includes 156 participants from 100 universities engaging in research projects remotely sponsored by the Boulder, CO and Gaithersburg, MD sites. This the first time that participants from both campuses have participated in the all activities collectively including the Colloquium. It's expected that the program will continue to grow in the future to include a virtual component while maintaining the in-person component. The nation's workforce is changing, and we must adapt.

During your attendance at the SURF Colloquium, I encourage you to interact with the SURF participants. In a virtual format, you may think the interactions are limited. Like the in-person program, there will be a Q & A period after each presentation. During this time, you're encouraged to ask questions using the chat feature, raise hand feature, or simply unmute yourself and verbally asking the question.
The colloquium is the perfect venue to exchange findings and new ideas from the most recent and rigorous research in all STEM fields.

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

Moreover, I invite you to share your colloquium experience on the National Institute of Standards and Technology (NIST) Facebook page using the hashtag, #2022SURFProgram.

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

Again, welcome to the Colloquium. I'm glad that you are spending your time with us and I hope you learn something new about the nation's standards laboratory.

Best regards,

Brandi K. Toliver

Brandi Toliver, Ph.D.

NIST SURF Program Managing Director

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NIST SURF Program Team

Organizational Unit (OU)	Name
Director's Office	Brandi Toliver
Director's Office	Kara Robinson
Communications Technology Lab	Linda Derr
Communications Technology Lab	Wesley Garey
Communications Technology Lab	David Griffith
Engineering Lab	Cartier Murrill
Engineering Lab	Shonali Nazare
Information Technology Lab	Lotfi Benmohamed
Information Technology Lab	Timothy Burns
Information Technology Lab	Yolanda Bursie
Information Technology Lab	Michaela Iorga
Information Technology Lab	Derek Juba
Information Technology Lab	Annie Sokol
Material Measurement Lab	Ilse Bercik
Material Measurement Lab	Tom Forbes
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	Joseph Dura
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
Advance Manufacturing	Lisa Fronczek

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Table of Contents

Summer Undergraduate Research Fellowship (SURF) Colloquium Plenary Session

Tuesday, August 2, 2022

Session Link: https://primetime.bluejeans.com/a2m/live-event/sgsskrrx

Time (EDT)	Session Information
10:00 AM	**Welcome (Jim Olthoff)**
	Session Moderator
10: 15 AM	**Communication Technology Laboratory (CTL)** Ovidio Castillo *Simulating the Impact of Manufacturing System Configurations on Production & Quality*
10:30 AM	**Engineering Laboratory (EL)** Catherine McCarthy *Ion specificity and the Hofmeister series in charged colloidal systems*
10:50 AM	**Information Technology Laboratory (ITL)** Ivy Liang *Interactive Online Histogram-Based Visualization of AI Model Fingerprints*
11:10 AM	**Material Measurement Laboratory (MML)** Yemi (Christine) Ogunsula *Building and Expanding the Drug DART-MS Forensics Database with Automated Tools*
11:30 AM	**NIST Center for Neutron Research (NCNR)** Jack Rooks *Particle orientation in soft materials from Small Angle Neutron Scattering*
11:50 AM	**Physical Measurement Laboratory (PML)** Lucy Yagodich *Interconnecting and Controlling In-Operando Spectroscopic Measurements*

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Tuesday, August 2, 2022 (1:00 to 2:30 PM (EDT))

	Engineering Laboratory (EL)	Information Technology Laboratory (ITL)	Material Measurement Laboratory (MML)
	Moderator: Helen Qiao	**Moderator: Tim Burns**	**Moderator: Kal Migler**
Time	Virtual Link: https://bluejeans.com/351211267/0730	Virtual Link: https://bluejeans.com/946424079/6073	Virtual Link: https://bluejeans.com/544223532/3099
1:00 PM	*Ainsley Rexford* Smarter Manufacturing: How images can help monitor thermal drift of machine tools	*Mitchell Campbell* Enhanced Viewing of 3D Objects Scanned using Photogrammetry	*Ryan Puthumana* Optimization of Clustering Algorithms for Small Angle Scattering of Polymer Formulations
1:15 PM	*Alex Dai* Integration of Neural Networks to Aid in Identifying Flame Temperatures	*Jason Eveleth* High-dimensional consensus mass spectra comparison	*Dennis Zhao* Analyzing Ternary Phase Diagrams Using Machine Learning
1:30 PM	*Arin Zeng* Optimizing Functionality of the Smart Target Data Collection System	*Ayush Varshney* Optimizing Data Communication for Low Latency Quantum Network Metrology	*Richard Ma* Improving robustness of active learning to accelerate XRD measurements of metal alloys using NMF
1:45 PM	*Diego Pantelis* Semantic Models for Building Systems	*Mikhail Krepets* Creating an Algorithm for Searching RNGs to Link with Test Results	*Maggie Hampson* Finite Element Modeling For Hydrogen Transportation & Storage
2:00 PM	*Dominique Paige* Development & Analysis of a Database of Tornado Impacts on Fire & Rescue Stations	*Miguel Lopez* Translating Mathematica Source Code to a Presentable LaTeX Format	*Aidan Knab* Machine Learning Automation of Charpy Impact Verification
2:15 PM	*Emily Liu* Premise Plumbing: Pressure Loss in Pipe Fittings and Water Quality Effect on Microbial Growth	[redacted]	*Brooke Calvo* Assessment of Shear Fracture Appearance in Charpy Specimens of Modern Steels
2:30 PM	Break		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session
Tuesday, August 2, 2022 (2:40 to 4:10 PM (EDT))

	Engineering Laboratory (EL)	Information Technology Laboratory (ITL)	Material Measurement Laboratory (MML)
	Moderator: Amanda Pertzborn	**Moderator: Ian Soboroff**	**Moderator: Becky Steffen**
Time	Virtual Link: https://bluejeans.com/351211267/0730	Virtual Link: https://bluejeans.com/946424079/6073	Virtual Link: https://bluejeans.com/544223532/3099
2:40 PM	*Emmy Smith* Additive Manufacturing Data Registration Software Development	*Samuel Rennich* Making TRECVID Results More Accessible and Coherent	*Charlotte Dohne* Creating Reference Libraries and STRBase Topic Pages on Emerging Areas in Forensic DNA
2:55 PM	*Eric Matthew Fagan* Structural Hardening for WUI Fire - Illustration Development	*Joshua Zarb* Understanding Neural Search Algorithms	*Jennifer Li* Characterization of Micrometer-Scale Particle Motion through Optimization of Analysis Parameters
3:10 PM	*Ethan Sundel* Using Standard Tests to Create a Public Drone Park	*Vaibhav Sanjay* Term and Relation Extraction in Mathematical Texts	*Grace Finch* Exploring Neutron Activation Analysis at the University of Maryland
3:25 PM	*James Timothy Allen* A Procedure for Implementing a Digital Twin	*Abishay Reddy* Multimodal Fusion with Modality-Specific Factors for IEMOCAP dataset	*Jacqueline Maloney* Evaluation of the Microscopy NexusLIMS Search Functionalities
3:40 PM	*John Gallo* Estimating Steady State Conditions of HVAC Systems	*Yuvan Sundrani* Artificial Intelligence-based texture analysis	*Terence Murphy* A Versatile Simulator for Cotranscriptionally Encoded RNA Strand Displacement Circuits
3:55 PM	*John Paul Alecia* Coordinated work as an aspect of Robotic Agility	*Robert Bao* Multimodal image registration for fluorescence guided surgery	*Nitin Elavarasu* Separation of composition from structure in Micro-X-ray fluorescence measurements
4:10 PM	Break		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Tuesday, August 2, 2022 (4:20 to 6:05 PM (EDT))

	Engineering Laboratory (EL)	Information Technology Laboratory (ITL)	Material Measurement Laboratory (MML)
	Moderator: Stephanie Watson	**Moderator: Derek Juba**	**Moderator: Ashlee Aiello**
Time	Virtual Link: https://bluejeans.com/351211267/0730	Virtual Link: https://bluejeans.com/946424079/6073	Virtual Link: https://bluejeans.com/544223532/3099
4:20 PM	*Jonathan Smilovich* Automation of Data Analysis for Rapid Characterization of Spectroscopic Imaging Maps	*Samuel Galita* Exploring Graph Analytics on Nisaba GPU cluster with cuGraph	*Bintou Koroma* The effect of randomness in branch spacing on LLDPE dilute solution properties
4:35 PM	*Joseph Fernandez* Graphic User Interface for ARIAC Robotics Competition	*Jaxon Ko* Benchmarking Queries from Zeno against FCPW	*Emily Frashure* Polymer Database Pipeline for the Circular Economy
4:50 PM	*Khoa Huynh* Object Recognition Framework for AR Interfaces	*Johannes Losert* Scientific Reproducibility of AI Trojan Detector Results	*Hrishikesh Ram* Interaction Energies of Zwitterionic Polybetaines with NaCl
5:05 PM	*Sin Lin* Developing Python script to facilitate ASTM C1556 Analysis of Bulk Concrete diffusion Coefficient	*Jane Liu* Implementing Real Time Constraints in Hedgehog API	*Marquesa Calderon* Analysis of existing NIST SRM for microplastics
5:20 PM	*Lindon Luu* Literature Review on Recreational Vehicle Fires		
5:35 PM	*Linsen Liu* Using Image Registration to Examine Melt Pool Monitoring Images.		
5:50 PM	*Mary Ruxsarash* Characterization of Components for a Pyrrhotite Reference Material		
6:05 PM	End of Day		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Wednesday, August 3, 2022 (10:00 AM – 12:00 PM (EDT))

	Engineering Laboratory (EL)	Information Technology Laboratory (ITL)	Material Measurement Laboratory (MML)
	Moderator: Xiaohong Gu	Moderator: Yolanda Bursie	Moderator: Ilse Bercik
Time	Virtual Link: https://bluejeans.com/351211267/0730	Virtual Link: https://bluejeans.com/946424079/6073	Virtual Link: https://bluejeans.com/544223532/3099
10:00 AM	*Noelle Crump* Validation Tests for the NIST Fire Dynamics Simulator	*Kyle Truong* Evaluating the Implementation of NIST SP 800-181 in Cybersecurity-Related Job Descriptions	*Leilani Meyers* Assessing Ambiguities in Metabolite Identification when Analyzed by LC-MS/MS
10:15 AM	*Oren Minsk* Measuring and improving the performance of industrial synergistic network	*Francis Durso* Addressing the Causes and Consequences of AI Failures	*Alexandra Terres* COMSOL Simulations of Contact Line Propagation in Additive Manufacturing with Ceramics
10:30 AM	*Owen Hammer* Mesh Optimization for AM Defect Detection Study using XCT Simulation	*Evelyn Hu* Dynamic Access Review and Control Implementation and Enforcement (DARCIE)	*Ross Gunther* Investigating Filament Fusion in Embedded 3D Printing
10:45 AM	*Robert Bennett* Deep Learning Applied to Industrial Robotics Simulation Environments	*Maggie Kristina Cavitt* Visualizing Cybersecurity Vulnerabilities and their Role in Recent Cyber Attacks	*Caressia Edwards* Atomistic Molecular Dynamics Analysis of a Model Polycarbonate/Silica Composite System
11:00 AM	*Robert Pang* A Biofidelic Impact Dummy to Evaluate the Safety of Collaborative Robot Applications	*Sheldon Douglas* Geometric augmentations to file identifiers in file system forensics	*Melissa A. Flores-Rivera* Structural Characterization of Extracellular Signal-Regulated Kinase 2
11:15 AM	*Sahil Kochar* Development of Web-based Service Life Prediction Tool for Photovoltaics and Building Materials		
11:30 AM	*Savannah Moldvay* Investigating Building Performance Using the Commissioning Software HVAC-Cx		
11:45 AM	*Tejas Nazare* Understanding the Evolution of "Sustainability" and "Resilience" in Literature		
12:00 PM	*Matthew Pham* Structural Stability Analysis: Application to 3D Printing of Cement-Based-Materials		
12:15 PM	Break		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Wednesday, August 3, 2022 (1:00 to 2:30 PM (EDT))

	Communication Technology Laboratory (CTL)	Physical Measurement Lab
	Moderator: Wesley Garey	**Moderator: Richard Steiner**
Time	Virtual Link: https://bluejeans.com/435534290/0420	Virtual Link: https://bluejeans.com/961384113/4619
1:00 PM	*Megan Lizambri* NetSimulyzer - A 3D Network Simulation Analyzer for ns-3	*Evan McClintock* Automating instrumentation for the calibration of DC power meters
1:15 PM	*Hannah Covington* Generating Realistic Residential Household Models of Varying Income Level for Simulations	*Samir Kulkarni* Simulating electron beam behavior in a miniature electron beam ion trap
1:30 PM	*Michael Belluscio* Applying Network-Enhanced GFCM to Characterize Grid Resilience	*Satvik Manjigani* Characterizing DNA Structures with Machine Learning
1:45 PM	*Aleysha Varghese* Assessment of Interoperability of Phaser Measurement Unit-Based Smart Sensors	*Shawn Meyer* Analysis of Dopant Quantum Dots in Silicon
2:00 PM	*Benjamin Philipose* Virtual Testing of ADS Equipped Vehicles	*Connor Lewis* Diffusion and Kurtosis in Brain Tissue Mimics
2:15 PM	*Prasun Guragain* Web API for visualizing data transference and vulnerabilities in systems	*Michael Gutowski* Computer Vision Identification and Analysis of Interferometric Fringes
2:30	Break	

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Wednesday, August 3, 2022 (2:40 to 4:10 PM (EDT))

	Communication Technology Laboratory (CTL)	NIST Center for Neutron Research (NCNR)	Physical Measurement Lab (PML)
	Moderator: Wesley Garey	Moderator: Dr. Guebre Tessema, National Science Foundation	Moderator: Uwe Arp
Time	Virtual Link: https://bluejeans.com/435534290/0420	Virtual Link: https://bluejeans.com/964520725/2477	Virtual Link: https://bluejeans.com/961384113/4619
2:40 PM	*Stephanie Estrella* Development and versions of standards repositories	*John Nunez* Revealing the magnetism of Weyl semimetal CeAlGe	
2:55 PM		*Shriya Haravu* Automatic Identification of Regions of Neutron Diffraction Patterns Changing During Phase Transition	*Michael Gabe* Nonperturbative nonlinear optics in a rubidium vapor cell
3:10 PM		*Benen Crombie* Automating the Fuel Element Visual Inspection Process at the NCNR Reactor	*Abrar Sheikh* Progress Towards Validation of the Cold-Atom Vacuum Standard
3:25 PM		*Washat Ware* Determining the validity of Guinier analysis in slit-smeared Small Angle Scattering data	*Nicolas Aguilar* Testing Calibration Uncertainty with Low-Cost Inertial Measurement Units with a Pendulum Method
3:40 PM		*Christopher Stallard* Developing a User-Friendly Framework for Stopped Flow Small Angle Neutron Scattering at the NCNR	*Joshua Young* Development of an Open-Source Workflow for End-to-End Simulation of an Ultrasonic Calorimeter for Imaging of Radiation Dose
3:55 PM		*Kim Taylor* Surfactant-Free Oil-in-Water Emulsion Stabilized by Chitin Nanocrystals: A Green Recipe	*Travis White* Metric Program Resource Development
4:10 PM		*Amy Musser* Multi-Scale Structures of Starch as Revealed by Scattering Techniques: From Unit Cell to Nanostructure	
4:25 PM	End of Day		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

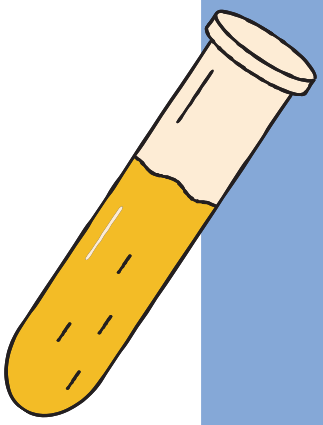
Thursday, August 4, 2022 (10:00 to 12:00 PM (EDT))

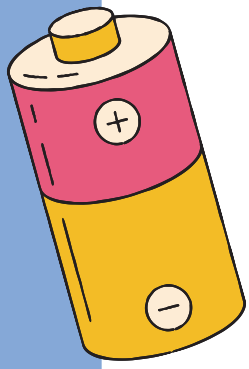
	Physical Measurement Lab (PML)
	Moderator: Uwe Arp
Time	Virtual Link: https://bluejeans.com/961384113/4619
10:00 AM	[redacted]
10:15 AM	*Faith Makumbi* Examining the Thermal Properties of an Artificial Star for Flux Calibration
10:30 AM	*Hunter Staiger* An automatic calibration algorithm and the efficiency determination of the NIST spectrometer
10:45 AM	*William Dienstfrey* Monitoring Atmospheric Stability for Plume Emission Flux Measurements
11:00 AM	*Aagam Dalal* Testing and demonstrating a new toolkit for public randomness beacons
11:15 AM	*Briana Chen* Developing resources for understanding an enhanced randomness beacon
11:30 AM	*Hayden Craun* Design of Multiresonant Plasmonic Nanocavities for Label-Free Nonlinear Optical Voltage Sensing
11:45 AM	*Gabriel Lewis* Normal Modes of Nanoscopic Ferromagnets
12:00 PM	Break

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Thursday, August 4, 2022 (1:00 to 3:00 PM (EDT))

	Physical Measurement Lab
	Moderator: Michael Berilla
Time	Virtual Link: https://bluejeans.com/961384113/4619
1:00 PM	*Helen Zhang* Hyperspectral Imaging for Tumor Margin Analysis in Breast Tissue Resection
1:15 PM	*Grace Tang* Evaluating Organic Thin-Film transistors and Processing Methods
1:30 PM	*Daniel Quinter* Quantum Random Number Generation in Trapped-Ion Computing with Error Mitigation
1:45 PM	*Max Buskirk* Analysis of Solder Joint Failures using Resistance Measurements
2:00 PM	**End of Colloquium**





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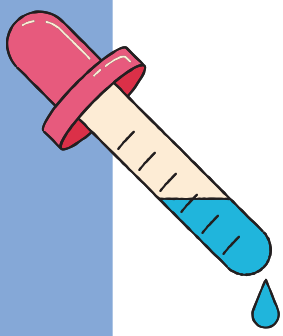

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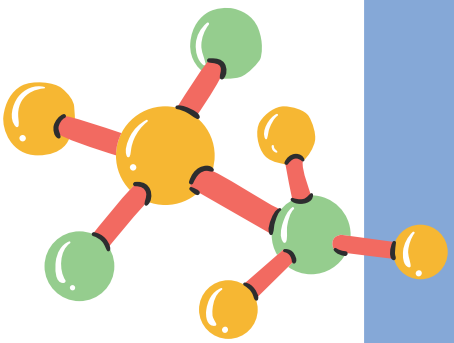
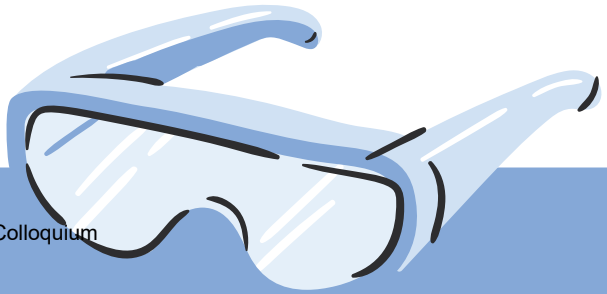




Summer Undergraduate Research Fellowship (SURF) - 2022 Participants

Communication Technology Laboratory (CTL)

Michael Belluscio

Ovidio Castillo

Hannah Covington

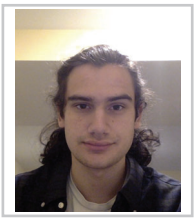
Stephanie Estrella

Prasun Guragain

Megan Lizambri

Benjamin Philipose

Aleysha Varghese



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Michael Belluscio	
Academic Institution: Purdue University	**Major:** Mathematics
Academic Standing (Sept. 2022):	Dean's List
Future Plans (School/Career):	To grad school for PhD in Mathematics, then to academia to research and teach.
NIST Laboratory, Division, and Group:	CTL, Smart-Grid Group
NIST Research Advisor:	Cheyney O'Fallon
Title of Talk:	Applying Network-Enhanced GFCM to Characterize Grid Resilience

Abstract:

Using the Generator Fleet Characteristics Model (GFCM) and only public data sources, we seek to characterize the resilience of large segments of the electric grid during major disturbance events that can lead to customer service interruptions. The network structure of the grid contributes to its resilience or lack thereof. We improve the GFCM through the development of a network module. We have created and implemented an algorithm we call “Prioritized Pathway” which creates synthetic connections between communities served by the electric grid based on spatio-temporal data of population and electric system operations. The algorithm creates synthetic networks of communities to lower the computational burden of generating more granular models, while also avoiding the need for sensitive and proprietary data on real world physical networks. We use this new module to construct network-derived cost adders that are incorporated into the existing model to deduce plausible hourly generator allocations. Furthermore, the summary statistics of the county level networks and data from the DOE-417, which details major electric system disturbances, are used to characterize a balancing authority’s resilience for every hour in a given year.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Ovidio Castillo
Academic Institution:	George Mason University
Major:	Systems Engineering
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Continue to Master's program
NIST Laboratory, Division, and Group:	CTL - Communications Technology Laboratory
NIST Research Advisor:	Michael Sharp
Title of Talk:	Simulating the Impact of Manufacturing System Configurations on Production & Quality

Abstract:

Optimization of production lines impact manufacturing quality and speed, and seeing configuration options in action provide manufacturers the ability to make informed, strategic decisions about their lines. Simulation tools are necessary to perform effective analysis of situations and configurations to better understand the systems and make educated decisions for positive impacts. The National Institute of Standards and Technology (NIST) maintains a simulation tool, Sim-PROCESD (Simulated-Production Resource for Operations and Conditions Evaluation to Support Decision-making), a PYTHON based software, to simulate different scenarios for manufacturing networks and help manufacturers make educated decisions to optimize their processes. The tool takes different production process configurations and simulates product quality and throughput as functions of increasing wear and degradation to the manufacturing equipment involved in the processes. It provides traceability of production systems and makes analysis faster and effective. The more elaborate the design becomes, there is longer production time, more issues arise and changes in quality occur. Research conducted shows there are limited amount of tools that can be used to automatically make random configurations of production networks. If the tool can make automation of configurations happen, in turn, it will give manufacturers more configurations to test and decrease planning time. There are situations where the manufacturer must test a configuration a certain way and there is no need for randomness or alternative designs. With sim-PROCESD, we can trace the paths and pin point defected machines and/or materials within the process to target the source of issues for decision making. With that, the tool helps information discovery capacity along with support in decision making. In the future, we want to be able to design configurations and help decrease production time by finding the best possible manufacturing line designs.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Hannah Covington
Academic Institution:	Santa Clara University
Major:	Mechanical Engineering
Academic Standing (Sept. 2022):	Graduate Student
Future Plans (School/Career):	I plan to pursue an M.S.M.E. degree at Santa Clara University
NIST Laboratory, Division, and Group:	CTL, Smart Connected Systems Division, Smart Grid Group
NIST Research Advisor:	Cuong Nguyen
Title of Talk:	Generating Realistic Residential Household Models of Varying Income Level for Simulations

Abstract:

Energy costs make up a significant portion of residential household expenditures. Developing innovations to decrease this cost involves rigorous testing. Testing using digital simulation is generally cheaper and faster than implementing products into actual homes. To support these simulations, it is crucial to create a method for quickly generating a multitude of realistic digital household models, each with varying house structure, occupant behaviors, and income level. Distinguishing between household income level allows innovators to ensure that their product promotes economic fairness across all users.

In order to inform the models, data had to be gathered about house characteristics, appliance usage, and occupancy patterns. Relevant data was gathered from the Residential Energy Consumption Survey (RECS), the American Time Use Survey (ATUS), and the U.S. Census. Surveyed households were then classified into one of five income levels based on their annual income, location, and number of household members. The data from surveyed households in each income level was then used to create probability distribution information for each of the model variables. For example, it is important to know the likelihood of an appliance being run a certain amount of times per week. Random number generation and the Monte Carlo method was employed alongside the probability distributions to determine the variables for each model. This information was inputted into the building energy simulator EnergyPlus to create the model and run simulations. The accuracy of the models was verified by running multiple baseline simulations and comparing the average energy consumption of the models with that of the surveyed households.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Stephanie Estrella		
Academic Institution:	University of Maryland, College Park	**Major:** Computer Engineering
Academic Standing (Sept. 2022):	Junior	
Future Plans (School/Career):	Obtain my undergraduate degree and then attend graduate school	
NIST Laboratory, Division, and Group:	Communications Technology Laboratory, Smart Connected Systems Division, Smart Connected Manufacturing Systems Group	
NIST Research Advisor:	Allison Barnard Feeney	
Title of Talk:	Development and versions of standards repositories	

Abstract:

The International Organization for Standardization (ISO), Technical Committee 184/Sub Committee 4 for Industrial Data, develops the Standard for the Exchange of Product model data (STEP). STEP, formally ISO 10303, is commonly used to exchange engineering design data in computer-aided design (CAD) systems with other CAD systems, with computer-aided manufacturing systems or coordinate measurement systems in manufacturing enterprises. STEP is a complex standard, composed of many inter-related parts. STEP developers rely on custom software to "build" the standards for ballot from technical content managed in a Git repository and presentation rules from the ISO Directives.

While participating in Task Force 1, STEP Module and Resource Library (SMRL) Architecture Innovation, I addressed ballot comments on the STEP Part 2 Vocabulary standard that is generated from the hundreds of source files in the STEP Module Resource Library. I generated my own Part 2 to check my work by installing a software environment that was helpful in adding, editing, and removing documents in Part 2. In Part 2 I went through checking for terms, in clause 3 (English definitions), that had duplicate term definitions which didn't follow the recommended ISO directives and rules, edited them to fit the ISO directives, but if they were very distinct to directive, I developed issues/tickets for these terms, then committed my current local repository with my changes. To commit, edit, and retrieve the repository from GitHub I learned commands from git. When installing the software development environment, many issues arose related to the configuration, so more research into tool installation was required. Through this experience I have learned the benefit of using git repositories for distributed development teams: you can effectively work on one part of the standard while others work on other parts and efficiently check errors or the change history. In the case of ISO standards, the ISO Directives which govern development and documentation of the standards are always changing. Being able to efficiently use git repositories will be worthwhile for other future standards or software development projects.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Prasun Guragain

Academic Institution: University of Wisconsin-Madison | **Major:** Computer Science

Academic Standing (Sept. 2022): Junior

Future Plans (School/Career): Graduate school

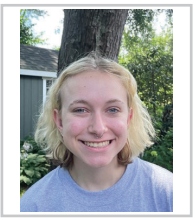
NIST Laboratory, Division, and Group: CTL, Smart Connected Systems Division, Smart Connected Manufacturing Systems Group

NIST Research Advisor: Allison Barnard Feeney

Title of Talk: Web API for visualizing data transference and vulnerabilities in systems

Abstract:

The current growth in the digitalization of businesses has been very beneficial, from better physical goods to faster services. However, due to increased reliance on digital data, they are exposed to many cyber threats, like data tampering. Data tampering is the act of changing data that is relied on by businesses. Tampering can be either intentional (i.e., cyberattacks) or unintentional (e.g., human or system error), which can lead to severe problems. Supply chains today are very complex, with many information systems running in the business. These system's tampered data can easily and quickly propagate across many other systems and into other businesses. Therefore, understanding and preventing the exposure of a business to such a threat is crucial. The Smart Connected Manufacturing Systems Group in the Communications Technology Laboratory at NIST is working on helping organizations quickly identify data integrity threats and propagation paths within their applications and network. The software solution, driven by security controls and activities defined in the NIST Cybersecurity Framework and NIST SP 800-53, allows users to: 1) build an inventory of their systems, applications, and networks, 2) be alerted of new vulnerabilities (from the NIST National Vulnerability Database - NVD) impacting their applications, and 3) understand and track all systems exposed (directly or not) to these vulnerabilities.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Megan Lizambri
Academic Institution:	University of Maryland, Baltimore County
Major:	Computer Engineering
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Complete my undergraduate degree, then enter a masters program in Computer Engineering. Ultimately obtain a job in the STEM field that challenges me both analytically and creatively
NIST Laboratory, Division, and Group:	Communications Technology Lab, Wireless Networks Division
NIST Research Advisor:	Evan Black
Title of Talk:	NetSimulyzer - A 3D Network Simulation Analyzer for ns-3

Abstract:

The increased complexity of network protocols and scenarios simulated using the discrete-event, packet-network simulator, ns-3, is making the development, verification, and analysis of simulations a challenging task. To aid in those tasks the NetSimulyzer, a flexible 3D visualizer for ns-3, was developed to alleviate the workload of debugging, understanding, and demonstrating a scenario. The tool was conceived to easily integrate into any ns-3 scenario and provides core functionalities that are technology agnostic. The NetSimulyzer provides mechanisms to track a variety of simulation elements, including the network topology and system performance that can later be visualized using a 3D scene augmented with data visualization elements, such as charts and logs.

This work presents a new feature implemented in the NetSimulyzer which allows for more detailed descriptions of individual elements of a wireless network simulation, as well as new and improved 3D models for the NetSimulyzer that were developed using an open-source, 3D modeling software, Blender. By shaping and combining basic geometry and coloring surfaces the new and improved models much more closely resemble the real-world items they represent and allow for additional information to be conveyed, while creating additional avenues for information facilitating the understanding of results. In conclusion, these efforts make for an enhanced user experience and further facilitate the development, verification, and analysis of simulations in ns-3.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Benjamin Philipose
Academic Institution:	Seattle University
Major:	Computer Engineering
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Pursue Masters Degree in Computer Science
NIST Laboratory, Division, and Group:	CTL, Smart Connected Systems Division, IOT Devices and Infrastructure
NIST Research Advisor:	Thomas Roth
Title of Talk:	Virtual Testing of ADS Equipped Vehicles

Abstract:

Vehicles equipped with Automated Driving System (ADS), for example, automated vehicles must be tested to ensure their safety and reliability to minimize the chance of a collision and to ensure their driving behavior matches human expectations. There is a need to develop new testing methods for safety metrics to support the Federal Motor Vehicle Safety Standards for ADS-equipped vehicles. The current trend in the automotive industry is towards confirming that ADS-equipped vehicles exhibit appropriate driving behaviors on the road to contribute to the overall safety of its passengers and the environment. NIST can contribute to this area of measurement science by developing methods of virtual testing that are fundamental to measuring the behavioral competency of ADS-equipped vehicles. For a testing environment, NIST has developed a software tool called the Universal Cyber-Physical Systems Environment for Federation (UCEF). UCEF is an environment that can be used to test ADS-equipped vehicles by manipulating their external factors to allow for a good virtual representation of a driving scenario. This work develops a testing framework for UCEF to define and run tests against the simulated automated vehicle which helps improve UCEF support for ADS-equipped vehicle testing. The driving simulation helps figure out what and how to measure behavioral competency by checking the automated vehicle's response to various driving scenarios. From the ADS-equipped vehicle's response, one can modify the testing framework over time. The testing software which interprets the response, SoapUI is connected to a car simulation that outputs data at each time step just as a normal car would. SoapUI takes this data from the car and checks, from current or previous responses, if the car is acting in a dangerous way. With this system in place, it allows for the efficient development of new measurement methods for assessing ADS-equipped vehicles' behavioral competency.

SURF Student Colloquium

NIST – Gaithersburg, MD

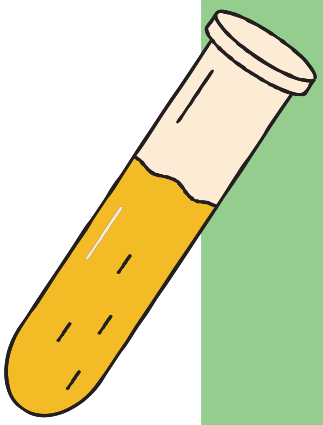
August 2-4, 2022

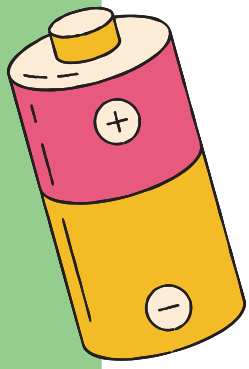
Name:	Aleysha Varghese
Academic Institution:	Virginia Tech
Major:	Computer Engineering
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Leadership in Corporate Technology
NIST Laboratory, Division, and Group:	Communications Technology Laboratory , Smart Connected Systems Division , Smart Grid Group
NIST Research Advisor:	Dr. Eugene Song , Kang Lee
Title of Talk:	Assessment of Interoperability of Phaser Measurement Unit-Based Smart Sensors

Abstract:

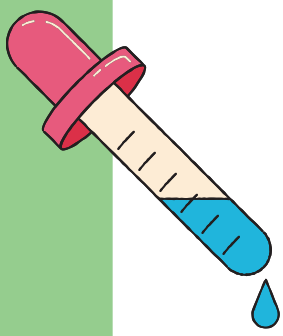
Smart sensors provide real-time data and the status of electrical power grids for monitoring, protecting, and controlling smart grids to improve their reliability and resilience. Smart sensor interoperability is a significant challenge for smart grids. Interoperability is the ability of two or more devices to use and exchange information through a standard protocol to achieve specific functions. To assure the interoperability of smart sensors in smart grids, a method for assessing needs to be developed and tested.

This project primarily focuses on the software tool development for interoperability assessment of smart sensors based on standard communication protocols, the model of interoperability, and the Hennessey-Milner logic. An open-source software tool is designed and developed in the Java programming language to automatically assess the interoperability of phaser measurement unit (PMU)-based smart sensors based on the Institute of Electrical and Electronics Engineers (IEEE) C37.118 standard communication protocol. This software tool parses the IEEE C37.118 packet dataset in extensible mark-up language (XML) format and automatically assesses the interoperability between phaser data concentrator (PDC) and PMU-based smart sensors. The assessment results are stored in a data file. These results determine whether the PMU-based smart sensors are inter-operable with PDC based on the IEEE C37.118 standard and provide an open-source software tool for any interested parties to use for interoperability testing of this specific smart sensor.





NIST | ENGINEERING LABORATORY



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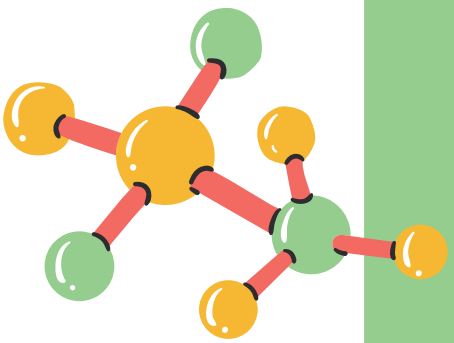
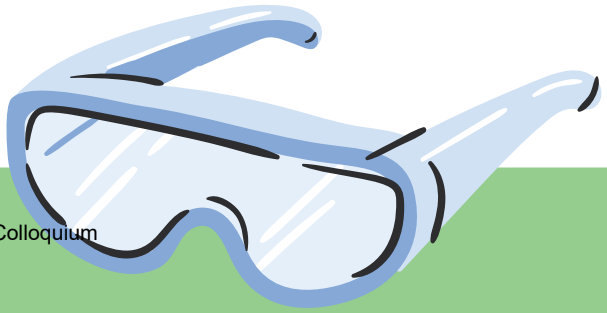




Summer Undergraduate Research Fellowship (SURF) - 2022 Participants

Engineering Laboratory (EL)

John Paul Alecia

James Timothy Allen

Robert Bennett

Noelle Crump

Alex Dai

Eric Matthew Fagan

Joseph Fernandez

John Gallo

Owen Hammer

Khoa Huynh

Sahil Kochar

Sin Lin

Emily Liu

Linsen Liu

Lindon Luu

Catherine McCarthy

Oren Minsk

Savannah Moldvay

Tejas Nazare

Dominique Paige

Robert Pang

Diego Pantelis

Matthew Pham

Ainsley Rexford

Mary Ruxsarash

Jonathan Smilovich

Emmy Smith

Ethan Sundel

Arin Zeng

SURF Student Colloquium

NIST – Gaithersburg, MD

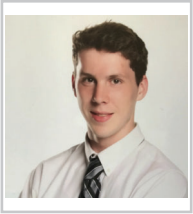
August 2-4, 2022

Name: John Paul Alicea	
Academic Institution: Benedictine College	**Major:** Mechanical Engineering
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Work in industry before going to graduate school
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Manipulation and Mobility System
NIST Research Advisor:	Anthony Downs
Title of Talk:	Coordinated work as an aspect of Robotic Agility

Abstract:

Robotic agility according to the Agile Robotics for Industrial Automation Competition (ARIAC) is defined as the ability to identify and recover from failures automatically, automate planning, minimize robot programming, reprogramming time, automate sensing within a fixture-less environment, and the ability to swap between robots of different manufacturers with minimal reprogramming time. During this competition, a system of two robots are programmed to perform different tasks. Utilizing the coordination between two robots maximizes the range and movement of a single robot and could improve planning and minimize programming time. Coordinated work between the gantry robot and the ground robot through software in the Agile Robotics for Industrial Automation Competition could yield a more agile and efficient robotic system overall. A new scoring factor for the Agile Robotics for Industrial Automation that would incorporate coordinated work between the robots must be created which would favor teams who utilized both robots during the competition.

In this study, two teams were selected that utilized both robots in the kitting portion of the 2021 ARIAC. The simulations of both teams were analyzed and the overall time of combined robot work for the respective trial and order was collected and used to create a new scoring factor. This scoring factor was used to yield new overall scores for the competition. In previous competition years, some teams would have yielded higher scores if this new scoring factor was implemented. Through the new scoring factor, which incorporates coordinated work between the two different robots, certain teams would have been rewarded more points, promoting the implementation of coordination as an aspect of agility during the competition. Implementing coordination between robots would yield a broader scope in measuring robotic agility and promote the utilization of both robots during competition trials.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: James Timothy Allen

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

Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Pursuing a career as a design engineer in smart industry or robotics
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group
NIST Research Advisor:	Dr. Guodong Shao
Title of Talk:	A Procedure for Implementing a Digital Twin

Abstract:

Recently, new technologies, such as machine learning and IoT devices, allow machines to collect and respond to real-time data in a meaningful way. These developments enable the realization of digital twins, which are fit-for-purpose, dynamic, and virtual representations of physical entities that are synchronized with their virtual entities. Using digital twins, conditions of the physical entity can be monitored, and optimal decisions can be derived to reduce costs and save time. However, it is still challenging for small and medium-sized enterprises (SMEs) to implement a digital twin due to the confusion surrounding the concept and lack of methodologies for implementing a digital twin.

In this project, a generic procedure for implementing a digital twin has been developed. This procedure provides a step-by-step guideline that aims to assist SMEs in development of their own digital twins. Machine health digital twins have been used to exemplify the proposed procedure. Predictive maintenance and anomaly detection cases of a computer numerical control (CNC) machine spindle are performed to identify relevant machine health issues and derive optimal decisions.

SURF Student Colloquium

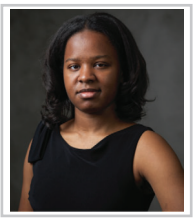
NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Robert Bennett
Academic Institution:	Bloomsburg University of Pennsylvania
Major:	Mathematics (Statistics Concentration)
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Graduate School : Georgia Institute of Technology : MS, Analytics ; Data Analyst->Data Scientist
NIST Laboratory, Division, and Group:	Engineering Laboratory (EL) Division 735, Intelligent Systems Division
NIST Research Advisor:	William Harrison
Title of Talk:	Deep Learning Applied to Industrial Robotics Simulation Environments

Abstract:

As industrial robotic systems become more complex, so does the process of teaching robots to perform desired tasks. Developing these agents (robots) to be intelligent could be conducive to learning efficiently, but the time and cost of learning on actual robots is substantial. Using 3D simulated environments to accomplish learning allows us to train agents more efficiently. In order for a robot to interact with its environment, a robot must be able to identify the locations of all objects in its environment as accurately as possible. This can be accomplished using pose estimation, a computer vision technique that tracks the locations of objects. The existing PoseCNN project successfully accomplished pose estimation of objects using only image data as input to a Convolutional Neural Network (CNN). The network estimates an object's pose by decoupling the estimation of 3D rotation and 3D translation. First, the 3D translation is estimated by localizing the center of an object and predicting the distance to its center. The 3D rotation is then estimated by regressing to a quaternion representation. This study seeks to assess how well PoseCNN performs using our own image data of manufacturing parts that might be present in robotics simulations. Additionally, this study analyzes the performance of the network on varying sizes of image data to understand to what degree accuracy is affected by the amount of training completed.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Noelle Crump	
Academic Institution: Worcester Polytechnic Institute	**Major:** Mechanical Engineering
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Finish Bachelors Degree in Mechanical Engineering
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Engineered Fire Safety Group
NIST Research Advisor:	Randall McDermott
Title of Talk:	Validation Tests for the NIST Fire Dynamics Simulator

Abstract:

The NIST Fire Dynamics Simulator (FDS) simulates fire spread behavior by producing the trends of values such as heat release rate, wind velocity, and temperature. A suite of test cases called validation cases use the simulator to replicate the conditions of a controlled burn done in a physical lab. The values produced by the physical and simulated burns are compared to test the accuracy of the simulator's values. A broad suite of these cases ensures the simulator can accurately recreate the progression of various fires. Two of the Validation test suites are the Memorial Tunnel and the Deep Fuel Beds test suites. The Memorial Tunnel validation suite tests FDS's capabilities to simulate tunnel fires. Few data sets of well-controlled full scale tunnel fires exist, and the standards for tunnel fire safety are not drawn from comprehensive testing. The Deep Fuel Beds suite tests FDS's ability to simulate burning vegetation with the Lagrangian Particle model. This validation case models the rate of flame spread depending on the spatial arrangement of discontinuous fuel beds.

Validating these cases includes writing scripts for automating tasks such as reformatting old and non-standardized experimental data, extracting the correct data from FDS, and processing the data for plotting the comparison. It also includes challenges such as deciphering old reports and finding the most accurate way to replicate the experiment. When a validation case runs cleanly, it is added to the tracked version of the FDS code on an online GitHub repository, assuring that this free public resource is working as intended.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Alex Dai

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

Academic Standing (Sept. 2022): Junior Year

Future Plans (School/Career): I plan on completing my undergraduate degree, then finding a stable job ideally close to where I live

NIST Laboratory, Division, and Group: Engineering Labratory, National Fire Research Laboratory, Un-supervised Learning in Fire Calorimetry Database

NIST Research Advisor: Prasad, Kuldeep

Title of Talk: Integration of Neural Networks to Aid in Identifying Flame Temperatures

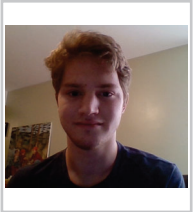
Abstract:

The NIST Fire Calorimetry Database has maintained thousands of experiments regarding the burning of common materials, each with at least one video in addition to a comma separated value sheet containing information regarding the fire. With this information, it is possible to train an artificial intelligence in order to identify the heat release rate of the flame without specific lab equipment. If successful, a video or photo of any situation may yield corresponding heat release rate information.

Because the information for the experiments are not easily publicly accessible, it was necessary to contact several staff members to gain access to the larger catalog of videos and corresponding files. Using the Python programming language and various libraries, we are able to extract frame data from the publicly available videos prior to this as a preliminary test. After the proof of concept succeeded, yielding a functioning neural network, we were able to move onto the private video files. Specifically, the neural network was constructed using Tensorflow-DirectML, and its corresponding keras libraries.

As a result, we were able to create multiple models with varying data sets and procedures, ultimately finding not only the best model to use, but also the best method to make such models, with each step carefully documented. With these models, an image may yield an estimate of the heat release rate of a fire captured in the image, or a video may yield a significantly more accurate representation of the heat release rate of any given frame.

If polished, not only can this be easily integrated into an application within a portable phone, security cameras can also warn staff of potential fires or hazards prior to an accident. Additionally, details regarding the construction of a neural network would undoubtedly be helpful for staff without the perfect hardware.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Eric Matthew Fagan

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

Academic Standing (Sept. 2022):	Junior undergraduate
Future Plans (School/Career):	Attend grad school for a master's degree in civil engineering and work for an engineering firm
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, Wildland-Urban Interface Fire Group
NIST Research Advisor:	Dr. Shonali Nazare
Title of Talk:	WUI Fire Structural Hardening - Illustration Development

Abstract:

Several components of a residential structure require fire hardening in order to prevent ignition from stray embers or flames, and this becomes increasingly important in areas where man-made and natural environments intersect - also known as Wildland-Urban Interface Areas. For example, a roof has many vulnerable components present. Debris in the gutters will dry out and ignite unless an noncombustible barrier prevents embers from getting through and vents can have dust and lint ignitions unless the flap is closed. Besides roof vulnerabilities, the eaves and siding can ignite from a nearby burning auxiliary structure. The Hazard Methodology and Mitigation document describes the various hardening actions that are required, the precedents (if any) in the existing code, and elaborates on the goals and methods of the actions taken. This way, homeowners and construction-centered businesses can make the modifications necessary for existing and new constructions in Wildland-Urban Interface communities and other high-hazard zones. However, the document is rather wordy, and as a result some critical information may be glossed over. Labeled illustrations effectively supplement text for readers to better understand the fire hardening modifications. To facilitate this, a compilation of illustrations highlighting modifications recommended in the Hazard Methodology and Mitigation document were prepared to form an appendix of the said document.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Joseph Fernandez
Academic Institution:	Salisbury University
Major:	Computer Science and Mathematics
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Attend gradutate school and pursue a career in computer science
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Cognition and Collaborative Systems Group
NIST Research Advisor:	Craig Schlenoff, Zeid Kootbally
Title of Talk:	Graphic User Interface for ARIAC Robotics Competition

Abstract:

The National Institute of Standards and Technology (NIST) Agile Robotics for Industrial Automation Competition (ARIAC) is a competition to test the agility of robots in the industry. Competing teams are given scenarios and objectives where they have to use the robots in the simulation to do kitting and assembly tasks. This competition helps to increase the agility of industrial robots, meaning they will be able to adjust to their environment even when unexpected changes occur.

To run a simulation for the competition, a Yet Another Markup Language (YAML) file needs to be input into the program. This text file gives Gazebo, the simulation software, the necessary parameters. In the past, the group trying to run a simulation would make their own file, which could lead to many errors. If any errors were present in the file, then the simulation would not run at all. The main goal of this project was to develop a graphical user interface (GUI) that creates the YAML file for the user and avoids potential errors that could occur when done by hand. This GUI reduced the amount of time taken to produce one of these files and also help eliminate errors.

After the interface was developed, a YAML schema was produced to check the output of the GUI to make sure that the outputted files are correct. Then the YAML files were checked for correctness by loading them into the simulation. Since the simulation would not run with an incorrect file, it was the best way that the output from the GUI was a correct and working file.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: John Gallo	
Academic Institution: University of Maryland	**Major:** Mechanical Engineering
Academic Standing (Sept. 2021):	Junior
Future Plans (School/Career):	Graduate in December 2022
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, Mechanical Systems and Controls Group
NIST Research Advisor:	Amanda Pertzborn
Title of Talk:	Estimating Steady State Conditions of HVAC Systems

Abstract:

The Intelligent Building Agents Laboratory (IBAL) is generating data on the performance of heating, ventilating, and air conditioning (HVAC) equipment. Some data sets are used to learn how to operate equipment or to understand the performance of equipment. Steady state data can be used to tune the operation of equipment and understand how it is performing under different circumstances. Steady state conditions are the final value of data after an infinite amount of time. Tuning is the process of modifying the input data (e.g., feedback from the system) through adding and multiplying values to change the output data (e.g., control signal for the equipment). This is required to ensure the output of the equipment matches the desired value.

In order to accurately predict the steady state value of each data set, the gathered data is fit to a function and evaluated as it approaches an infinite running time. After an infinite time, the data should converge to a finite value. This allows the function to guess a final value without requiring an infinite data set. The accuracy of this function depends on how closely it follows the trend of the original data.

I have been tasked with creating a MATLAB script to predict the steady state values for any data set. The estimation I've created functions based off of an exponential function with a decreasing rate. This allows the estimation to extend past the given data to approximate what the final value of the data would be if allowed to continue infinitely. Most of my work has been writing and optimizing the code to accurately and efficiently run the script to predict steady state values of each data set. The final version of the code can be used by researchers to process data sets of any size.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Owen Hammer

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

Academic Standing (Sept. 2022): Junior

Future Plans (School/Career): Attend Graduate School

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

NIST Research Advisor: Felix Kim

Title of Talk: Mesh Optimization for AM Defect Detection Study using XCT Simulation

Abstract:

Additive manufacturing (AM) is a very effective technique that can have a major impact upon the manufacturing industry, but defects in metal AM are preventing wider adoption of the technique. Several X-ray Computed Tomography (XCT) defect detection algorithms are being developed to resolve this issue, but it is challenging to evaluate their performance due to the lack of ground truth information of physical samples. Using XCT simulations with a voxelated surface mesh representing pores in the metal is important because they can produce benchmark data and eliminate uncertainty that would be present in ground truth image data. A mesh is a representation of a three-dimensional object with a series of points and two-dimensional shapes that connect them. In this study, a program was developed to generate surface meshes that follow voxel boundaries as this capability is not readily available in existing libraries. Two major functions were written: one that creates a voxelated mesh surface from a three-dimensional binary image, and another that converts a triangulated mesh surface into a three-dimensional binary image. These algorithms can be used together to voxelate a mesh, which is then used in an XCT simulation with randomly positioned pores. Three major methods of surface meshing, along with their advantages and disadvantages are discussed. The algorithm that converts a mesh in a stereolithography (.stl) file to three-dimensional voxel image and its capabilities are displayed. The usage of these functions in a larger program that simulates randomly positioned pores is then shown. Using procedural voxelated mesh generation allows for a more efficient, cheap, and accurate method for XCT AM defect detection simulations. Opportunities for optimization of these algorithms and modification and application of the overall program to other problems will be discussed at the end of the colloquium.

SURF Student Colloquium

NIST – Gaithersburg, MD

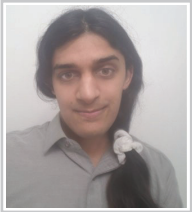
August 2-4, 2022

Name: Khoa Huynh		
Academic Institution: University of Maryland, College Park	**Major:** Computer Science	
Academic Standing (Sept. 2022):	Junior	
Future Plans (School/Career):	Graduate School	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Sensing and Perception Systems Group	
NIST Research Advisor:	Shelly Bagchi	
Title of Talk:	Object Recognition Framework for AR Interfaces	

Abstract:

Manufacturing processes have become increasingly sophisticated, which has led many manufacturers to use robotics to enhance the speed, quality of production and complete many complicated tasks. However, in small and medium-size enterprises (SMEs), tasks change quite frequently so collaborating robots has become an important part of a successful and sustainable SMEs. However, controlling and operating a robot currently requires sophisticated knowledge of each robot and takes time to learn.

To enable non-technical users to operate and work with robots, the Performance of Human-Robot Interaction (P-HRI) project at NIST aims to create an Augmented Reality (AR) system to enable human-robot collaborative tasks in manufacturing environments. An integral part of this AR system is object recognition that can identify parts and indicate which is the next-needed part in the task. The goal of our project was to create an object recognition framework that can integrate into AR interfaces for interactions between humans and robots. Using the program Unity along with the C# programming language, we created an app with Vuforia's object detection to be able to pick out an object through the camera view. This allows the end user to see the object highlighted with AR annotations while interacting with their environment. We also experimented with openCV and Python to create a color detection framework but the accuracy of Vurforia's object detection provided higher accuracy and lower time to detection. The end goal of this project is to integrate the object recognition framework into AR headsets for a more seamless experience.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Sahil Kochar		
Academic Institution: University of Maryland College Park	**Major:** Aerospace Engineering + Mathematics	
Academic Standing (Sept. 2022):	Recent Graduate	
Future Plans (School/Career):	TBD	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Infrastructure Materials Group	
NIST Research Advisor:	Dr. Xiaohong Gu	
Title of Talk:	Development of Web-based Service Life Prediction Tool for Photovoltaics and Building Materials	

Abstract:

Many kinds of polymers are used for solar photovoltaic (PV) systems. Yet the polymers chemically and mechanically degrade under their service environments with ultraviolet (UV) light, temperature, and humidity. In order to properly design solar panels and ensure warranties, it is critical that the PV industry is capable of efficiently assessing the long-term performance and lifetime of their materials is critical. The primary focus of my research this summer is to develop a user-friendly web tool comprised of physics-based statistical models that can describe the effects of key environmental factors on degradation, accelerated laboratory tests to real-world performance for backsheet polymeric materials. The statistical model uses a cumulative damage model which has been effective at predicting the chemical degradation of a commercial PV backsheet, with changes that allow it to more directly predict changes in mechanical degradation. In particular, the total UV exposure on a model PV backsheet material is correlated with the material's ductility, as measured via the elongation-at-break of specimens. The model is developed into an R Shiny web tool that allows users to quickly fit the model's parameters to a specific backsheet material and compare the model's predictions with measured data, providing significant value to companies that wish to design and/or test solar installations.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Sin Lin

Academic Institution: University of Virginia | **Major:** Civil & Environmental Engineering

Academic Standing (Sept. 2022): Fourth-Year

Future Plans (School/Career): Pursue Master's degree in environmental engineering

NIST Laboratory, Division, and Group: Engineering Laboratory (EL)

NIST Research Advisor: Aron Newman

Title of Talk: Developing Python Script to Facilitate ASTM C1556 Analysis of Bulk Concrete Diffusion Coefficient

Abstract:

The concrete industry is one of the largest global consumers of natural resources, and as sustainability continues to become more prominent in the construction community, focus is shifted to the service life of a concrete structure. As it degrades – either by chloride (Cl) induced corrosion of the steel reinforcement or external sulfate attack -- the structure is repaired or replaced many times, which has a proportional effect on the environment. The diffusion rate of a deleterious species from the environment into the concrete largely controls the structure's service life. To reduce this diffusion rate is to reduce the degradation rate, thus increasing service life. According to ASTM C1556, the apparent Cl diffusion coefficient, D, for hardened cementitious mixtures can be determined using a representative sample of the mixture that is separated into a test specimen and an initial Cl-content specimen. The test specimen is sealed (except for one exposed face), saturated, and placed in a sodium chloride solution for a specified exposure time. After it is removed, layers are ground into a powder, one-by-one, to determine the Cl content of each. The apparent Cl diffusion coefficient is estimated from the concentration values that are measured at each depth while using the surface and background internal concentration as adjustable parameters. Then, the measured Cl- contents are fitted to the concentration function of interest. The aim is to develop a software script that uses non-linear regression analysis and the error function to estimate the D coefficient that results in a curve best-fitted to the observed data. The values in ASTM C1556 were used to verify the script, but one of the objectives is to allow the user to provide an independent estimate for the adjustable parameters. Thus, the optimal parameters and uncertainties that allow for increased service life of the concrete structure can be promptly provided.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Emily Liu
Academic Institution:	University of Maryland, College Park
Major:	Civil Engineering
Academic Standing (Sept. 2022):	Sophomore GPA
Future Plans (School/Career):	Industry
NIST Laboratory, Division, and Group:	Engineering Laboratory/ Building Energy and Environment Division (BEED)/Mechanical Systems and Controls Group
NIST Research Advisor:	Natascha Milesi Ferretti and Tania Ullah
Title of Talk:	Premise Plumbing: Pressure Loss in Pipe Fittings and Water Quality Effect on Microbial Growth

Abstract:

Premise plumbing distributes cold and hot water to consumers in buildings such as homes. The system consists of pipes, fittings, valves, fixtures, and appliances (e.g., water heaters). Pipes and heaters should be properly sized and operated not only to prevent energy losses, but also long periods of stagnant flow, which can create conditions for the growth of pathogenic microorganisms. Data is lacking to characterize premise plumbing that is more reflective of present building water usage and modern pipes and fittings to improve efficiency, safety, and public health. The objective of this SURF project was to assist two ongoing projects at NIST. For the first project focused on plumbing hydraulics at the cold-water distribution, a database was created by extracting information on pressure loss coefficients (i.e., an important pipe sizing parameter) from literature for pipe fittings. Using this database, visualization of the data was accomplished by developing Python scripts to create graphs comparing the Reynolds number and other flow parameters to pressure loss coefficients. Through the findings in the literature review and data processing, relationships between the analyzed parameters were observed. The second project was focused on water quality measurements in a hot water system. The objective was to extract information from manuals on the installation, calibration, and operation of sensors in a real-time monitoring instrument used to measure chemical and physical water quality parameters in a water heater laboratory test setup. By understanding the parameters measured and conducting a literature review, the potential effect of water quality on microbial growth in water heaters was studied.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Linsen Liu

Academic Institution: University of Maryland	**Major: Applied Mathematics**

Academic Standing
(Sept. 2022): Sophomore

Future Plans
(School/Career): Graduate School

NIST Laboratory,
Division, and Group: Laboratory:Engineering Lab Division: 734-System Integration Division
Group: 734.12 Information Modeling and Testing Group

NIST Research
Advisor: Dr. Yan Lu

Title of Talk:

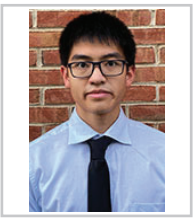
Abstract:

One of the prominent technical challenges powder-bed-fusion Additive Manufacturing process faces is process variability and the resulting part-quality issues. This project investigates process monitoring methods based on melt pool imaging. Various feature extraction methods are applied to the melt pool images captured from the NIST Additive Manufacturing Metrology Testbed (AMMT) for process anomaly detection. In addition to assessing features from individual MPM images and performing anomaly detection based on individual features, such as melt pool size and shape, this study focuses on examining melt pool variations by registering adjective melt pool images and extracting multiple features for process fault detection and diagnosis. The advantage of the proposed method is that different melt pool features are sensitive to different process abnormalities during a build. For example, the melt pool size can reflect the total energy absorbed from the laser; the melt pool orientation may indicate the deviation of a scan path. Measuring several features could lead to more efficient detection and minimization of process variability due to the increased specificity of information conveyed by each feature.

This study gathers and analyzes the melt pool images collected from the NIST AMMT. The data set is a set of coaxial melt pool images (relative static melt pool, follows optical path) with a small field of view of $120\ pixel \times 120\ pixel$. The pixel size is 8 micrometers. The images are sampled at 10 kHz. The normal scan speed is 800mm/sec.The study uses an ellipse fitting method to collect the features of MPM images such as melt pool center location, melt pool width, melt pool height, melt pool orientation, melt pool area, perimeter, circularity, and aspect ratio (ratio between width and height of non-rotated fitted rectangle). The next step is to compare consecutive images for melt pool center, angle of rotation, circularity, and aspect ratio and calculate the percentage changes. To implement the algorithms, the study used Python with OpenCV, NumPy, Matplotlib, and Pandas. The study deploys the fitEllipse function to fit a melt pool boundary based on the least square method, along with the boundingRect function to find the aspect ratio. Finally, layerwise statistical features as mean, standard deviation, maximum, and minimum are calculated for both the features itself and the changes.

The results of this study are summarized in two sets of data: one containing the nine features for individual MPM and one containing the changes of these features. The study has also generated statistics of these two sets in order to better understand the data set. Preliminary results indicate several features have strong sensitivity to irregular melt pool. The study expects more results for direct image registration method to compare the accuracy and efficiency.

This study proposes an innovative process control method based on image processing and registration. It indicates that multiple features can help effectively control the process by more specific fault indications. One preliminary conclusion that can be drawn is that image processing with an emphasis on the change between adjacent images gives more useful information than image processing based solely on the characteristics of the images themselves.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Lindon Luu		
Academic Institution:	University of Maryland, College Park	**Major:** Fire Protection Engineering
Academic Standing (Sept. 2022):	Undergraduate Junior	
Future Plans (School/Career):	Graduate School	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, WUI Group	
NIST Research Advisor:	Shonali Nazare	
Title of Talk:	Literature Review on Recreational Vehicle Fires	

Abstract:

Structural ignitions and structure-to-structure fire spread within Wildland-Urban Interface (WUI) communities during wildfire can occur by direct flame impingement, ember exposure, thermal radiation, and combinations thereof. WUI fire case studies have identified multiple sources that can directly cause structure ignitions. The sources include combustible fences, wood piles, combustible landscaping elements, storage sheds, auxiliary structures, non-commercial vehicles, and recreational vehicles (RVs). Structure Separation Experiments (SSE) project addresses structure-to-structure fire spread in the WUI communities. Phase 1 of the SSE project quantified fire hazard from storage sheds while Phase II will address quantification of fire hazard from recreational vehicles (RVs) and non-commercial vehicles. In preparation for the forthcoming experiments on RV fires, this project focused on reviewing literature on vehicle fires overall, and to analyze published data including peak heat release rate(PHRR), temperatures, smoke release, and mass loss rate. The experimental set-up, the instrumentation information, and test procedures including sources and locations of ignition were reviewed.

The understanding of the burning behaviors of several vehicles including the sedans, minivans, and heavy goods vehicles(HGV's) facilitated estimation of the RV fire hazards. Analysis of the HRR data from literature revealed PHRR ranging from 1.9 MW to 202 MW for the vehicle fires and showed a positive linear correlation between the mass of a vehicle and the PHRR. The estimated PHRR of the RV used in the upcoming experiments is expected to be in the range of 28 MW ± 10 MW given that the RV mass will vary approximately between 2485 kg ± 100 kg. The temperatures recorded during vehicle fires typically ranged from 900°C to 1300°C. Analysis of RV fire statistics indicated that the most common area for the origin of a fire was the engine, the running gear, and the wheel area and that the ignition occurred due to worn-out wires or friction that generated intense heat.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Catherine McCarthy	
Academic Institution: Georgetown University	**Major:** Physics
Academic Standing (Sept. 2022):	Graduated
Future Plans (School/Career):	Physics PhD at the University of Massachusetts, Amherst
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division (MSSD), Infrastructure Materials Group
NIST Research Advisor:	Abhay Goyal
Title of Talk:	Ion specificity and the Hofmeister series in charged colloidal systems

Abstract:

Charged colloidal systems, a class of materials that ranges from biological membranes to hydrated cement, contain charged nanoparticles suspended in an aqueous ionic solution. Cohesive forces between these charged particles arise due to the formation of hydrated-ion structures that dramatically reduce the dielectric screening capacity of water. This effect becomes most pronounced at high confinement. Since the size and geometry of the hydrated-ion structures depend on the size and valency of the ionic species, the cohesive forces in charged colloidal systems are naturally ion specific as well. We use semi-atomistic Monte Carlo and Molecular Dynamics simulations of cationic counterions and explicit water molecules confined between charged surfaces in order to investigate the role of ion specificity in charged colloidal systems. We find that the interplay of ion size and valency, in combination with the complex manner in which those factors interact with the surface charge density and confinement, is responsible for differences in the nanoscale structure and cohesive forces of systems with different species of counterions. Furthermore, for highly charged, dense systems, we link the magnitude of the cohesive force between colloidal particles in systems with different species of counterions to the order of the Hofmeister series and discuss the various aspects of ion specificity that contribute to the order.

*This research was supported by the Hichwa Fellowship at the Georgetown University Department of Physics, the Clare Boothe Luce Program, and the NIST SURF Program.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Oren Minsk

Academic Institution: University of Pennsylvania

Major: Mechanical Engineering

Academic Standing (Sept. 2022): Sophomore

Future Plans (School/Career): Undecided, likely will pursue masters degree in some engineering field

NIST Laboratory, Division, and Group: Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group

NIST Research Advisor: Dr. Nehika Mathur

Title of Talk: Measuring and improving the performance of industrial synergistic networks

Abstract:

The circular economy is a paradigm for a more sustainable economy in which raw materials from the Earth have a cyclical life that involves them being shared, repaired, reused, and recycled. Industrial symbiosis is a process where byproducts or waste of one manufacturing firm are used as feedstock by another firm, and therefore industrial symbiotic networks play crucial roles in facilitating a circular economy by reducing our dependence on natural resources and mitigating supply chain risks. Only one large and efficient industrial symbiotic network has existed for a number of decades, and it's located in Kalundborg, Denmark. This project focuses on an industrial network of transactions, mainly in Ohio, and aims to provide recommendations for how it can be improved, with the motivation of increasing the presence of industrial symbiosis in American manufacturing. The network is manipulated to experiment with how different real-life modifications could potentially improve the n twork. These modifications include observing the network transactions year-by-year, duplicating the network, and adding hypothetical nodes and edges. Social network analysis is implemented in an attempt to quantify the improvements made by the modifications compared to the baseline network. Metrics including density, a number of centrality measures, and network efficiency are calculated, analyzed, and used to gain understanding of the network and aforementioned modifications. Breaking down the Ohio network year-by-year reveals that almost no transactions were made in multiple years, suggesting that involvement and retention are challenges. Existing literature aligns with our findings and would suggest improving personal relationships between firm managers and increasing use of similar materials by firms.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2022

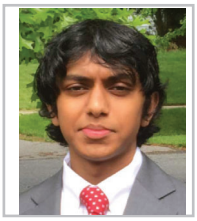
Name: Savannah Moldvay	
Academic Institution: University of Maryland, College Park	**Major:** Civil Engineering
Academic Standing (Sept. 2021):	Sophomore
Future Plans (School/Career):	Purse a career in Civil Engineering
NIST Laboratory, Division, and Group:	Engineering Laboratory, Building Energy and Environment Division, Mechanical Systems and Controls Group
NIST Research Advisor:	Michael Galler, Natascha Milesi-Ferretti
Title of Talk:	Investigating Building Performance Using The Commissioning Software HVAC-Cx

Abstract:

Owners of large Commercial buildings, such as college campuses, are investing millions of dollars for heating, ventilation, and air-conditioning (HVAC) systems. The expectation for these systems is to consistently operate and function efficiently with minimal energy waste. Yet, many are performing inadequately. This leaves employees operating in less than ideal work environments, building owners paying larger energy bills, and huge productivity losses because of inefficient HVAC systems.

As a response, this project seeks to improve the performance of HVAC systems by identifying and addressing equipment performance faults. Michael Galler and Natascha Milesi-Ferretti developed the HVAC Commissioning (Cx) tool at the National Institute of Standards and Technology (NIST). HVAC-Cx is a semi-automated commissioning software tool designed to assist in the analysis of HVAC systems in commercial buildings. This software conducts its analysis through detecting faults related to improper operation, which are then illustrated through detailed graphs. These graphs are then incorporated in the documentation of the final results.

For this project, we were able to review HVAC data from both NIST and the Robert E. Parilla Performing Arts Center (PAC) at Montgomery College. The data we received is analyzed by HVAC-Cx to test the performance of the HVAC systems. This evaluation is formed into a final report and helps inform the building owners of the system's current operation. From the PAC, we currently have a short period of time in which data was evaluated. This brief amount of data causes difficulty in assessing the full operation of the HVAC system. Therefore, in the future we plan to obtain larger spans of data. Yet, at this time we have analyzed the available PAC data from January 11th to February 24th of 2022. From this period, data was collected from multiple components of the HVAC system. A few examples of the types



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Tejas Nazare
Academic Institution:	University of Maryland, College Park
Major:	Economics/Mathematics
Academic Standing (Sept. 2022):	Rising sophomore
Future Plans (School/Career):	Pursue graduate studies in economics, enter industry or research
NIST Laboratory, Division, and Group:	Engineering Lab, Applied Economics Office
NIST Research Advisor:	Dr. Jennifer Helgeson
Title of Talk:	Understanding the Evolution of "Sustainability" and "Resilience" in Literature

Abstract:

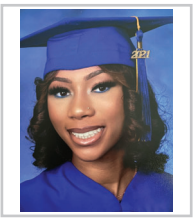
The climate crisis has been characterized by climate change, erratic weather patterns, environmental degradation, and increasing food insecurity. According to the United Nations website, climate change is a major threat to international peace and security. Climate change has been brought to a forefront in politics, popular media, and scientific research in recent years. Consequently, research on strategies to combat the crisis has increased significantly.

Two major concepts are at the heart of this research — sustainability and resilience. The terms have been used with increasing frequency and consist of a significant segment of recent literature. This project takes on a structured literature review and analysis of trends in the study of sustainability and resilience.

The methods of this research included a systematic review of the use of these terms in the literature and in the popular press. The Web of Science database was used to conduct an analysis of the use of the terms across disciplines. Using the Web of Science platform and Matlab, code was developed to create insightful visualizations regarding the number of pertinent papers, distribution amongst scientific categories, and citation/reference numbers. Furthermore, I augment this analysis with analysis using Lexis-Nexis and the NSF grants manager search engine to better understand the extent to which these areas are being studied (through funded grants) and communicated to the public.

I found that since 2012, both sustainability and resilience have become highly cited in the literature, with resilience following sustainability. In addition, the study of sustainability has evolved from being somewhat evenly distributed amongst categories to being heavily centered on environmental sciences and green and sustainable science technology. The study of resilience has expanded from primarily environmental fields to other fields, such as psychiatry.

The study of sustainability and resilience will become increasingly pertinent as the world searches for ways to endure and mitigate the climate crisis. Cognizance of these terms is critical to evaluating the nature and direction of this research.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Dominique Paige	
Academic Institution: Morgan State University	**Major:** Cloud Computing
Academic Standing (Sept. 2021):	Sophomore
Future Plans (School/Career):	Tech Job
NIST Laboratory, Division, and Group:	Engineering Lab, Materials and Structural Systems Division, Structures Group
NIST Research Advisor:	Marc L. Levitan & Nico de Toledo
Title of Talk:	Development & Analysis of a Database of Tornado Impacts on Fire & Rescue Stations

Abstract:

Despite the severe threat that tornadoes pose, there is still much to learn about how they affect critical facilities in the United States. Due to the high likelihood of collapsed structures and other emergencies after a tornado, it is crucial that fire, rescue, and emergency medical services stations are not damaged. While other studies have documented the impacts of specific tornadoes and tornado outbreaks on fire, rescue, and emergency medical services stations, there is still a gap in knowledge about the cumulative national impact of tornadoes on these critical facilities. To fill this gap we are creating a database of these impacts by mining National Weather Service tornado narratives from the National Centers for Environmental Information's Storm Events Database. Our database covers United States tornadoes from January 1993 through February 2022. The mining process consists of filtering all the narratives for ones that describe a tornado striking the property of a fire, rescue, or emergency medical services stations and then extracting details about the impact.

First, we generated a list of keywords, like "fire" and "squad," in an effort to discover every case when tornado impacts on fire, rescue, and emergency medical services stations were mentioned. We tested and refined the list of keywords to limit the number of false positives. We used the keywords to filter the narratives in Microsoft Excel and then read through each narrative to see if one of these facilities was indeed hit by a tornado. If so, we recorded details including a description of the damage, the station name, and station coordinates.

This database will aid in decisions about whether to require tornado-resistant engineering design standards and/or storm shelters in fire, rescue, and emergency medical services stations to ensure that these critical facilities are able to provide emergency services after a tornado.

SURF Student Colloquium

NIST – Gaithersburg, MD

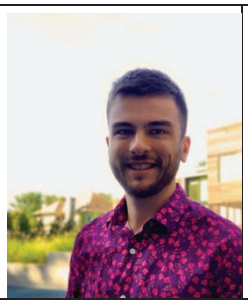
August 2-4, 2022

Name: Robert Pang		
Academic Institution: University of Maryland College Park	**Major:** Mechanical Engineering	
Academic Standing (Sept. 2022):	Junior	
Future Plans (School/Career):	Finish bachelor's degree at UMD	
NIST Laboratory, Division, and Group:	Engineering Laboratory	
NIST Research Advisor:	Kenny Kimble, Joe Falco	
Title of Talk:	A Biofidelic Impact Dummy to Evaluate the Safety of Collaborative Robot Applications	

Abstract:

As technology advances, work in the manufacturing industry is automated by robots more and more. Collaborative robot systems allow humans and robots to work more closely to create a more efficient workflow. Collaborative robots need to be tested in order to determine their safety before being allowed to be used in a collaborative environment. ISO/TS 15066 provides a list of biomechanical limits on force and pressure for various body parts in case of human-robot impact. Testing with real humans is dangerous and risks harm, so a safety test dummy should be used instead. The test dummy should mimic the mass properties, mechanics, and anthropometry of the human body. The test dummy design should be repeatable, easy to manufacture, easy to set up, easy to use, easy to calibrate, and minimize cost.

A dummy design based on an accurate model of a 50th percentile male, (determined by the US National Highway Traffic Safety Administration (NHTSA) THOR automotive crash dummy) is leveraged. Each region of the body is designed and tested separately beginning with the right forearm, then completing the arm, and eventually the entire body. The forearm and upperarm have been designed and tested, validating the process and results of the design. The design and implementation of a hand is next. If pressures at each location are below a corresponding threshold, the robot may be approved.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2022

Name: Diego Pantelis

Academic Institution: University of Maryland College Park | **Major:** Bioengineering

Academic Standing (Sept. 2022): Junior

Future Plans (School/Career): I plan to pursue a career in biomedical instrumentation

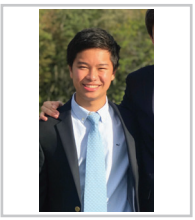
NIST Laboratory, Division, and Group: Engineering Laboratory, Building Energy and Environment Division, Mechanical Systems and Controls Group

NIST Research Advisor: Parastoo Delgoshaei

Title of Talk: Semantic Models for Building Systems

Abstract:
Being able to use building system information for analytics, automation and control is essential in the effort to achieve energy-efficient buildings. The building systems that will be needed to achieve national goals for energy-efficient, grid-integrated buildings lack interoperability and machine readability of information. To address this issue, there are current efforts to create a standard for semantic building modeling that will allow for fault detection and diagnostics (FDD), system optimization and automation on a broader scale. These efforts aim to create formal models that represent building components and their relationships, including the data that is produced from such a system (sensors, control switches, etc.). These standards use technologies such as Resource Description Framework (RDF), Web Ontology Language (OWL), and SPARQL Protocol and RDF Query Language (SPARQL) in order to establish such models.

The first step of this summer's research is the modeling of the heat pump laboratory at NIST using the standard draft's concepts and methodology. It is modeled based on schematics that include the topological connection between the equipment. Consequently, a series of queries are developed for an FDD application. The goal of this research project is to create a model that can be used as a case study that provides feedback for the development process of the standard and improves the validation procedure. The project essentially allows for a real-world example of what a building's model using the current standard draft would look like in the hope of giving the standardization effort insight into the current standard's flaws.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Matthew Pham
Academic Institution:	University of Maryland
Major:	Mechanical Engineering
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Pursue a career as a mechanical engineer
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems Division, Inorganic Materials
NIST Research Advisor:	Dr. Nicos Martys
Title of Talk:	Structural Stability Analysis: Application to 3D Printing of Cement-Based-Materials

Abstract:

Concrete is one of the oldest and the most widely used building materials. Despite it's history of usage, there is interest in making it more sustainable, reducing its impact on the environment and in developing new ways of placing it. Recently, new technologies based on 3D printing have been developed that have the potential to revolutionize the process of placing concrete. 3D printing is less labor intensive and allows for more possibilities in architectural design. For a new technology to be accepted, standards and guidelines have to be developed for it's usage that insure the quality of construction.

In this research project we investigate the stability of certain structural designs that may typically be 3D printed. We varied the geometry of structures as well as investigated the tolerance for stability based on small variation in its placement and different applied forces. We also examine what minimum material properties are required to maintain the stability of various structures.

We utilized commercial software to design and compute the response of structures to external forces as a function of design and material properties such as Young's Modulus, Poisson's ratio, and density.

The results of these studies provide insight to the geometrical constraints as well as material properties necessary to perform a successful 3D print.

SURF Student Colloquium

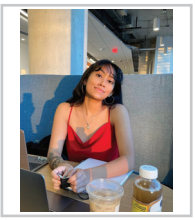
NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Ainsley Rexford
Academic Institution:	University of Pennsylvania
Major:	Mechanical Eng. and Applied Mechanics
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Most likely pursue a masters degree in product design or robotics.
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Production Systems Group
NIST Research Advisor:	Gregory W. Vogl, PhD.
Title of Talk:	Smarter Manufacturing: How images can help monitor thermal drift of machine tools

Abstract:

Precision manufacturing is increasing in importance as manufacturers seek to make their processes faster and cheaper while still producing quality parts. A major hurdle in the quest for precision machining is thermal drift, which can account for up to 70% of machining accuracy errors. This study focuses on developing and testing a new method to monitor the thermal drift of machine tools using videos of dot calibration grids taken with a high-magnification wireless microscope. To do this, a dot calibration grid is fixed at each corner of the machine tool worktable and a wireless microscope camera is mounted in the tool holder of the spindle. Since the machine tool can move in three dimensions (X, Y, and Z) and the spindle can rotate, videos with various types of machine motion can be captured and analyzed to determine the thermal drift of the spindle relative to the worktable. Next, these videos are parsed into images to segment the dots and track the individual X and Y dot center positions. The Z dot position is estimated by finding the Z position that yields the maximum contrast of dot edges. The tracked positions are then inputted into a two-dimensional (X and Y) or three-dimensional (X, Y, and Z) linear model to solve for the 2D or 3D changes within the machine tool. For example, the 2D model contains six thermally induced variables that are solved in a least-squares manner: X translation, Y translation, Z rotation, XY squareness change, and XY planar thermal growth coefficients. Experiments were conducted to test the ability of this new technique to measure commanded translations as large as 50 micrometers. Data analysis revealed that this method was accurate at a micrometer-level and is an effective way of measuring thermal drift. Overall, a relatively cheap wireless microscope and small calibration grids can be used to track thermal drift in near real time. Such an approach has significant future commercial potential for diagnosing and correcting thermal drift in machine tools which will advance manufacturing precision and efficiency.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Mary Ruxsarash

Academic Institution: American University **Major:** Chemistry

Academic Standing (Sept. 2022): Junior

Future Plans (School/Career): PhD, Graduate School

NIST Laboratory, Division, and Group: Engineering Lab

NIST Research Advisor: Stephanie Watson

Title of Talk: Characterization of Components for a Pyrrhotite Reference Material

Abstract:

Damage to residential and commercial concrete structures in Connecticut have been attributed to the oxidation of the iron sulfide mineral pyrrhotite. Sulfates that are released from pyrrhotite oxidation react to cause internal sulfate attacks and further expansions, contributing to long-term concrete cracking and crumbling. There are currently no standardized test methods to assess pyrrhotite occurrence and abundance in aggregate or in concrete. Therefore, developing a standard test method and a set of calibration reference standards is crucial in curating an accurate and consistent analysis of pyrrhotite in concrete.

This project aims to assess and quantify the content of pyrrhotite in concrete foundations by developing reference materials, characterizing major mineral species in these reference materials, and determining consistent and effective standard test methods for pyrrhotite analysis. The reference material consists of a representative aggregate, Ottawa sand, and hydrated cement that can be mixed into various concentrations to create calibration curves for pyrrhotite measurements. We've approached testing the material with two methods: X-ray fluorescence (XRF) and X-ray diffraction (XRD). The data was analyzed for mineral composition using various methods and programs, such as Highscore, Profex and Microsoft Excel. This project will offer a valuable glimpse into developing a standard test method, including a set of calibration reference standards, which will provide a means for accurate and consistent analysis of pyrrhotite in concrete.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Jonathan Smilovich

Academic Institution: The City College of New York | **Major:** Environmental Engineering

Academic Standing (Sept. 2022): Senior

Future Plans (School/Career): MBA Graduate School

NIST Laboratory, Division, and Group: Engineering Lab

NIST Research Advisor: Dr. Stephanie Watson

Title of Talk: Automation of Data Analysis for Rapid Characterization of Spectroscopic Imaging Maps

Abstract:

Molecular spectroscopic techniques, including Fourier Transform Infrared (FTIR) and Raman spectroscopies, have made advancements using microscopy to collect spectroscopic maps of specific locations for chemical structure identification for materials applications. These spectroscopic maps can contain thousands of spectra, which can take many hours to process and analyze. Furthermore, each spectrometer vendor requires a unique macros or automation script to process (i.e., baseline correct, normalize and peak ratio) each series of spectra. Consistent data processing is essential to effectively track chemical changes in materials with our laboratory aging experiments. We would like to create a general script or series of scripts to process spectra from FTIR and Raman spectral maps using Python or other programs that can be applied to multiple instruments. This project focused on Raman mapping of photovoltaic backsheet materials. OPUS was used to extract the spectral data from the Raman maps. Baseline correcting is then applied to remove any background noise and align the spectra measurements. Origin was then used to normalize the data and implement methods to quantify the chemical changes with degradation. Improving efficiency of this process is the main focus of this project. Automation of selecting spectra, baseline correcting, and normalizing was then performed. OPUS Macros have been utilized in combination with elements of Python to automate the process. The automation script would then allow any spectral file to be efficiently analyzed. The output then consists of mapping the peaks of the various spectra for further analysis.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Emmy Smith		
Academic Institution: The University of Alabama in Huntsville	**Major:** Industrial/Systems Engineering & Math	
Academic Standing (Sept. 2022):	Graduated	
Future Plans (School/Career):	Graduate School	
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Information Modeling and Testing Group	
NIST Research Advisor:	Dr. Shaw Feng	
Title of Talk:	Additive Manufactuirng Data Registration Software Development	

Abstract:

Laser-powder bed fusion processes for metal Additive Manufacturing allow for more flexibility in metal component manufacturing. The quality of these parts needs to be observed and studied to ensure components meet design requirements for the targeted applications. The quality is determined through the amount and size of defects, or air pockets, present in the metal. The goal of this study is to take X-ray Computed Tomography images of the metal and develop software to determine the defects present. The main focus is creating ground truth images for artificial intelligence. The ground truth images will be used as baseline images for artificial intelligence training through U-NET. This method completes image segmentation which groups images based on their values and assigns them to classes. The ground truth images will train the images to recognize the classes that are defects.

These ground truth images are created through a process of image segmentation and thresholding. The defects appear as dark spots and the algorithm detects dark areas and creates a rectangular bounding box that contains the entire dark area. These boxes are then used with a thresholding algorithm to determine the defects. This thresholding is run with multiple thresholding methods like Otsu. The new images with the specific boundaries are then compared to the originals. The images that are found to be accurate maps are selected as ground truth for the machine learning baseline.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2022

Name: Ethan Sundel

Academic Institution: University of Pennsylvania | **Major:** Mechanical Engineering

Academic Standing (Sept. 2022): Sophomore

Future Plans (School/Career): Finish my bachelor's degree and pursue a master's degree

NIST Laboratory, Division, and Group: Engineering Laboratory, Intelligent Systems Division, Emergency Response Robots and Drones

NIST Research Advisor: Adam Jacoff

Title of Talk: Using Standard Tests to Create a Public Drone Park

Abstract:

NIST is creating a set of standardized test methods to quantify the performance of emergency response drones as well as pilot proficiency. First responders can use these standard tests to train and measure their ability to fly unmanned aerial vehicles in emergency scenarios. NIST's main aerial tests include apparatuses that are inexpensive and easy to fabricate created from wood and plastic buckets. They are constructed in specific manners to ensure that they test the pilot and drone on proficiency in many different areas.

The first part of this project was for me to learn about NIST's current aerial tests and learn how to proctor them in order to gain perspective into how the tests function. I was given the opportunity to travel to a robotics competition as well as a STEM camp which allowed me to gain firsthand experience proctoring these tests. Along with proctoring, by the end of the summer I will have obtained a few different credentials including FAA Safety Team Certificate for the NIST Open Test Lane, FAA remote pilot license (Part 107), and Airborne Public Safety Association (APSA) Advanced Proctor Certificate for NIST Open and Obstructed Test Lanes and Scenarios.

The end goal of this project is for me to design a more durable version of NIST's tests. This version of the tests will create a public drone park in Philadelphia, Pennsylvania. By creating a more durable version of the tests using different materials, they will be able to withstand all weather conditions for an extended period of time, with little to no maintenance required. As drone technology advances, more pilots are being credentialed by the FAA in order to increase the use of drones in emergency response scenarios. This drone park will serve as an effort towards helping local first responders and anyone else in the Philadelphia area measure their proficiency and improve their skills in the field.

SURF Student Colloquium

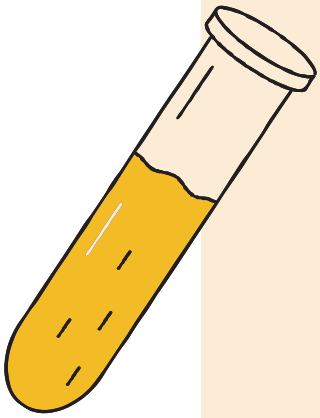
NIST – Gaithersburg, MD

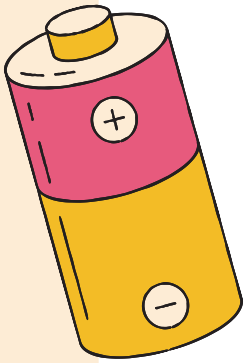
August 2-4, 2022

Name: Arin Zeng	
Academic Institution: University of Maryland College Park	**Major:** Computer Science
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Earn a B.S in Computer Science and Applied Math
NIST Laboratory, Division, and Group:	Engineering Laboratory
NIST Research Advisor:	Helen Qiao
Title of Talk:	Optimizing Functionality of the Smart Target Data Collection System

Abstract:

Recently, the use of robots in high precision tasks have greatly increased such as 3D printing, automated manufacturing, robot assembly, etc. This has presented a challenge in keeping the robots performing these tasks precise and at high quality. The smart target detection system uses computer vision to recognize the positions of objects using a 6D (points and vectors) measurement system. This technology is useful in detecting mechanical degradation in robots. Currently, the industry best practice to fix degradation is to conduct local calibrations or in process inspection to confirm that degradation has not occurred to the extent to damage robot quality. The smart target vision system aims to improve maintenance responsiveness of the robot to maintain a higher quality of robot health. The smart target object is viewed through two camera lenses to determine its position. Functions to load in preset camera parameters and to identify the positions of each colored (red, green, blue) lines were added. The goal and task is to optimize performance of this tool and to debug the software tools of the Smart Target Data Collections program. Adding the individual color detection lines and loading preset camera parameters in will make it easier to collect data and measurement. The purpose is to increase the efficiency of measurement and improve the technology transfer to industry. Having a computer program that is able to accurately and efficiently detect the positions of objects that have the smart target sensor will help humans maintain the quality of robots and effectively prolong the healthy performance of the robots.





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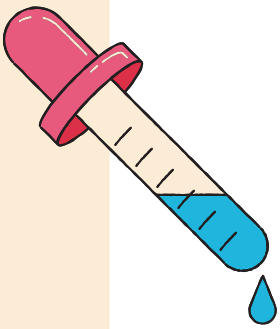
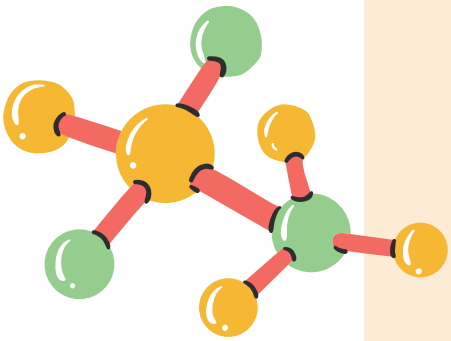
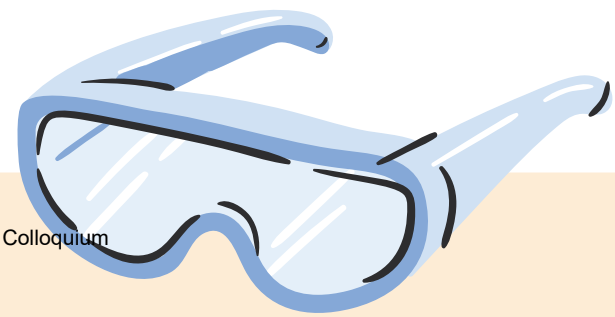


2022





Summer Undergraduate Research Fellowship (SURF) - 2022 Participants

Information Technology Laboratory (ITL)

Robert Bao

Mitchell Campbell

Maggie Kristina Cavitt

Sheldon Douglas

Francis Durso

Jason Eveleth Samuel

Galita Evelyn Hu

Jaxon Ko

Mikhail Krepets

Ivy Liang

Jane Liu

Miguel Lopez

Johannes Losert

Abishay Reddy

Samuel Rennich

Vaibhav Sanjay

Yuvan Sundrani

Kyle Truong

Ayush Varshney

Joshua Zarb

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Robert Bao	
Academic Institution: University of Illinois at Urbana-Champaign	**Major:** Computer Engineering
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Attend graduate school
NIST Laboratory, Division, and Group:	PML/ITL
NIST Research Advisor:	Peter Bajcsy, Maritoni Litorja
Title of Talk:	Multimodal image registration for fluorescence guided surgery

Abstract:

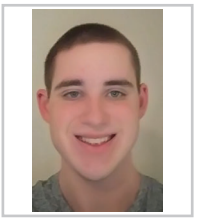
Fluorescence guided surgery is an important tool for surgeons to accurately identify and remove cancerous tumors. This work is motivated by the spatial misalignment of real-time streaming brightfield images and fluorescent images with tumor indications acquired by a fluorescence guided hand-held imaging system during a head and neck surgery. The spatial misalignment of brightfield and fluorescent images pose challenges for a surgeon who is deciding where to remove tumor tissue with significant consequences for a patient.

The problem of spatially aligning (registering) two multimodal images involves designing an automated method for estimating registration transformation parameters. The challenges include (a) achieving high spatial accuracy for tumor tissue removal, (b) overcoming limitations of existing algorithms that are optimized for monomodal images and assume many spatial features in both modalities and (c) decoupling the intermodality transformation and registration tasks in multimodal algorithms .

We approached the multimodal registration problem by (a) creating ground truth data by manually registering paired images (b) evaluating the effectiveness of traditional image registration algorithms such as SIFT, and (c) training and testing an unsupervised generative adversarial network (GAN) called NeMAR. The NeMAR method consists of a spatial transformation (registration) network, intermodality translation network, and discriminator network.

By testing different configurations of NeMAR with artificially generated training images, training iterations, and network types, we found the optimal NeMAR configuration with respect to our ground truth registered images. The method's accuracy increases with the number of input image pairs, but remains about the same for over 200 epochs of training.

In summary, while machine learning methods show promise in multimodal registration tasks, a robust GAN-based method would require a large training dataset sampling from a variety of surgical environments. Future research will compare a supervised machine learning approach to our unsupervised GAN-based approach with more training data.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Mitchell Campbell

Academic Institution: Virginia PolyTechnic Institute and State University | **Major:** Computer Science

Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Plan on pursuing a career in software development after obtaining my Bachelor's degree.
NIST Laboratory, Division, and Group:	Information Technology Laboratory
NIST Research Advisor:	Sandy Ressler
Title of Talk:	Enhanced Viewing of 3D Objects Scanned using Photogrammetry

Abstract:

Most of a museum's collection is held in storage due to a lack of space for public displays. One solution for displaying these stored artifacts is to create 3D models of them. This can be done using photogrammetry, a technique for creating 3D virtual models of objects by taking many pictures of an object from different angles and using software that inputs camera images in order to reconstruct a virtual model mesh. These models are then saved as glTF files. glTF (GL Transmission Format) is a file format used to store 3D models and scenes, and is becoming an ISO (International Organization for Standardization) standard.

This study focuses on features that can be implemented to improve the user experience of viewing imported glTF models. Implemented features are presented to the user as a series of tools that can be interacted with through an on-screen HUD (heads-up display). Some of these tools include a light that follows the mouse cursor to brighten a model and annotations for describing individual parts of a model. Annotations are presented to the user through a separate HUD window that appears when clicking on an object. All tools were developed in AFRAME, a web framework that uses HTML and Javascript to create 3D scenes which are viewable through a web browser and virtual reality devices.

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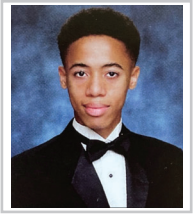
NIST – Gaithersburg, MD

August 2-4, 2022

Name: Maggie Kristina M. Cavitt		
Academic Institution: ECPI University	**Major:** CIS (Cybersecurity)	
Academic Standing (Sept. 2022):	Junior	
Future Plans (School/Career):	My goal is to obtain a graduate degree and work on high-performance or quantum computer research.	
NIST Laboratory, Division, and Group:	Information Technology Lab (ITL)	
NIST Research Advisor:	Hung Trinh and Katherine Schroeder	
Title of Talk:	Visualizing Cybersecurity Vulnerabilities and their Role in Recent Cyber Attacks	

Abstract:

The influx of recent large-scale cyber-attacks has created the need to understand how known cybersecurity vulnerabilities impact the integrity, availability, and confidentiality of network infrastructures across all business and government sectors. To aid in cybersecurity awareness efforts the NIST and its team of researchers are working to furnish the cybersecurity community with well-informed datasets/metrics. The goal if this project is to capture the process of enhancing cybersecurity related data through a wide range visualization software and resources. Utilizing the NIST's National Vulnerability Database (NVD), a breakdown of verified cyber vulnerabilities with each vulnerability's criticality score and influencing factors, we can identify some of the most common types of network/system vulnerabilities. Together with additional open-source resources such as CISA, the U.S. Department of Health and Human Services Office for Civil Rights, and others we can establish multipoint connections and create approximate reference relationships between the NVD's vulnerability data and a significant number of reported cybersecurity incidents. From these connections we are then able to create visualizations that depict the correlations and possible influencing factors between many of the published vulnerabilities and recent incidents/breaches. By utilizing multiple data visualization services like PowerBI, Splunk, and ElasticSearch we can then create unique visualizations and compare similar findings from across the different services to validate the results. Once we are able to complete this process, we can then apply a method for tagging the data that will assist information security personnel and developers in determining how to prioritize implementing patches for these vulnerable systems.



SURF Student Colloquium

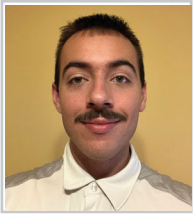
NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Sheldon Douglas
Academic Institution:	University of Maryland, College Park
Major:	Computer Science
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	To pursue a master's degree in computer science leading to a career in software engineering or cyber security.
NIST Laboratory, Division, and Group:	Information Technology Laboratory
NIST Research Advisor:	Alexander J. Nelson
Title of Talk:	Geometric augmentations to file identifiers in file system forensics

Abstract:

Digital forensics is a process that is key to examining and interpreting data in cyber related investigations. File system forensics makes up a significant portion of digital forensics as it is logically sorting through hard drive storage to determine creations, deletions, and other data essential to event reconstruction. Important to the functionality of file systems is the principle of namespace uniqueness, which uses file paths and names as identifiers that can distinguish file objects. In the world of digital forensics, there are several libraries used, one being, The Sleuth Kit (TSK). Within it is a command, 'fiwalk', whose purpose is to convert raw disk images' metadata into extensible markup language (XML) but does not populate with the guarantee of namespace uniqueness due to its reporting of unallocated ("deleted") files. This reporting of unallocated files means that file names cannot be relied on as identifiers. Considering the need to review unallocated files, logical code changes that focus on incorporating new identifiers for file objects are made necessary. This work evaluates a practice that identifies: the start of an index node (a file's attributes), the start of the directory entry, and the start of the file's content, producing a three-dimensional address for each file object. Subsequently, reported results from a 2012 paper that contain a measurement discrepancy will be corrected and additionally, this research will enable better cross-tool comparison.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

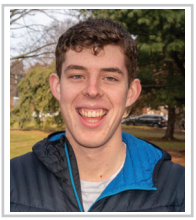
Name:	Francis Durso
Academic Institution:	Johns Hopkins University
Major:	Computer Science
Academic Standing (Sept. 2022):	Full-Time Student, Junior
Future Plans (School/Career):	Software Developer / Programmer / Cyber-Security Consultant
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division
NIST Research Advisor:	Dr. Raunak and Dr. Kuhn
Title of Talk:	Addressing the Causes and Consequences of AI Failures

Abstract:

Artificial Intelligence (AI) has become increasingly prevalent in nearly all areas of life. It now controls our thermostats, drives our cars, produces our electronics, recognizes our faces, evaluates our resumes, predicts our purchases, and so much more. But what happens when AI systems fail, and how can we learn from these failures to prevent such incidents in the future? Our project proposes a framework for characterizing these AI failure incidents, and provides a structured way of documenting them in an online repository.

This repository is designed to address some key concerns. First, it will provide all known, verifiable information about the AI failure incidents in a convenient, searchable manner to allow users to discover and learn about these incidents with some level of technical depth. Secondly, it will allow users to report incidents as new ones are discovered, ensuring that the data remains up to date. Lastly, it will address the issue that Machine-Learning based AI systems tend to be black boxes. While such systems often succeed in achieving remarkable levels of accuracy, they rarely provide much understanding of their decision making process or the factors that influence its decisions. Our proposed characterization of the AI-failures will help us gather information that could shed light on this aspect.

Regular software vulnerability documentation efforts, such as NIST's National Vulnerability Database (NVD), require some knowledge about the inner workings of the code to be analyzed effectively. Such details are a lot harder to garner when it comes to AI/ML failures. Our proposed framework - Failures of Artificial Intelligence Learning Systems (FAILS) - captures the causes for the incident, the sources of weaknesses involved, and a measure of impact that the failure caused without needing to know the details of the code. In short, all the information needed to ensure it doesn’t happen again.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Jason Eveleth	
Academic Institution: Brown University	**Major:** Math-Computer Science
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Pursue a PhD in math or computer science
NIST Laboratory, Division, and Group:	ITL, Applied and Computational Mathematics Division, Mathematical Analysis and Modeling
NIST Research Advisor:	Dr. Anthony Kearsley
Title of Talk:	High-dimensional consensus mass spectra comparison

Abstract:

Mass spectrometry (MS) is an analytical chemistry technique for analyzing compounds. It provides a signature--called a mass spectrum--that can be used for compound discrimination. That signature is a scatterplot of charged fragments of the substance. One popular application is forensics chemistry, where drug chemists are trying to determine whether seized evidence is an illicit drug.

The traditional method for discriminating mass spectra in forensic chemistry is to bin the scatterplot into a vector (essentially a histogram) and take the cosine similarity between the vectors. While generally effective, this method can occasionally lead to misidentifications. We recently developed two novel methods for incorporating measurement variability when comparing mass spectra to limit the likelihood of misclassifications.

The first method works by binning the mass spectra--identical to the traditional approach--but then uses the mean and standard deviations of the bins across replicate measurements to form a summary-statistic vector. The second method works by taking the n highest y-valued points in the mass spectra and finding the mean and standard deviation across replicate measurements of that value and using the statistics to represent the compound. We use these summary-statistics as a more informative way to compare compounds.

We have implemented these methods in C and performed preliminary evaluation using experimental data collected with two different types of mass spectrometers. We have found good performance in the discrimination of current drugs of interest (methamphetamine vs phentermine, nicotinamide vs isonicotinamide) and are currently evaluating the performance of these new methods across a larger test set of mass spectra that are difficult to discriminate by the traditional method, including applications outside of seized drugs.

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NIST – Gaithersburg, MD

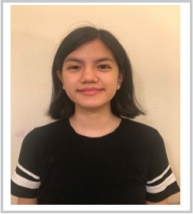
August 2-4, 2022

Name: Samuel Galita	
Academic Institution: University of Maryland	**Major:** Finance & Mathematics
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Considering a career in data science or quantitative finance
NIST Laboratory, Division, and Group:	Information Technology Laboratory
NIST Research Advisor:	Min Ding
Title of Talk:	Exploring Graph Analytics on Nisaba GPU cluster with cuGraph

Abstract:

Graph algorithms and Graph analytics are designed for manipulating and analyzing graph types of data to determine the relationships between graph objects and the structural characteristics of a graph as a whole. They have been adopted and used heavily in fields such as social networking, route optimization, fraud detection, and so on. A major issue with modern graph analytics is that it is usually challenging to perform the algorithms quickly or with high computational efficiency at a large scale. Graphics Processing Units (GPUs) can be utilized to accelerate graph data analysis and machine learning. Recently, NVIDIA produced the open-source graph analytics library cuGraph, which operates directly on GPU DataFrames and provides a collection of GPU accelerated graph algorithms with NetworkX-like API that can be treated as an efficient graph analytics solution for Python users.

The purpose of this project is to evaluate benchmark graph analysis algorithms on NIST's Nisaba GPU cluster and compare the quantitative performance of cuGraph with other CPU-based graph analysis tools, such as NetworkX and NetworKit. Both synthetic and real world datasets are employed to benchmark the common network analysis algorithms among six categories, namely Katz for centrality analysis, Louvain for community detection, Breadth-First-Search (BFS) and Single-Source-Shortest-Path (SSSP) for graph traversal, Weakly Connected Components for component detection, and PageRank for link analysis. Furthermore, cuGraph supports multi-GPU and multi-node operations (MNMG) in conjunction with Dask (Dask cuGraph). Dask cuGraph was also benchmarked alongside cuGraph and NetworkX. Through our reproducible experimentation, we were able to identify large performance increases when using the cuGraph library compared to both NetworkX and NetworKit, as well as unprecedented scalability of graph analytics using multiple GPUs. A GitLab repository was created to allow future users to test the cuGraph benchmarks with their own specifications and provide implementation examples for using the library.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Evelyn Hu
Academic Institution:	UC Berkley
Major:	Computer Science
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Graduate with a bachelor's degree and pursue a career in technology
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Computer Security Division
NIST Research Advisor:	Dr. Michaela Iorga and Nikita Wootten
Title of Talk:	Dynamic Access Review and Control Implementation and Enforcement (DARCIE)

Abstract:

As cloud services are becoming more widely adopted, the amount of data available to members of an organization is vastly increasing along with the risk of data breaches.This project develops an access control mechanism that dynamically reviews, implements and enforces access control policies in real-time. The mechanism ensures granularity of control through privilege access management, allowing the system to control user access to resources. The access control mechanism enforces zero-trust policies so that users are continuously authenticated and are granted or denied access to the sensitive information based on their geolocation, organization's network availability and historic pattern of accessed resources.

Our proof-of-concept system uses two devices to simulate a user accessing local or cloud data. A virtual machine acts as the end user's device and another device acts as a router that simulates different geolocations from where data in the cloud is accessed. The system demonstrates a dynamically changing policy generated by the state of a sensor and enforced by the kernel using Security-Enhanced Linux (SELinux). In this case, the demo system limits a user's access to some system resources based on the device's connection to an access point, simulating a dynamically generated access policy based on geographic location. Future work will focus on access control policy review and control implementation and enforcement rules also derived from the user's historic pattern of accessing the resources of interest.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Jaxon Ko

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

Academic Standing (Sept. 2022): Senior

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, Software and Systems Division, Information Systems Group

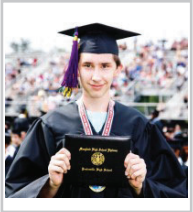
NIST Research Advisor: Derek Juba

Title of Talk: Benchmarking Queries from Zeno against FCPW

Abstract:

NIST has developed a software called Zeno, which estimates material properties from a geometric model of a particle of said material. One of the main computational tasks Zeno performs is to compute the closest point on the model to a query point. In addition, a newly proposed algorithm in Zeno would need to determine whether a part of a geometric model is contained within another. Currently, Zeno uses an internally-developed library to compute its closest point queries. However, using another open-source library may prove to be more optimal. In this project, we benchmark the closest point and contains queries performed by the current Zeno library against those performed by the "Fastest Closest Points in the West" (FCPW) library. The results of these benchmarks will help us decide whether or not the internally-developed Zeno library should be replaced with the FCPW library when implementing the new Zeno algorithm.

To obtain the benchmarks, we created C++ programs using either library. Users can specify a .obj file for the program to construct its geometric model, a query type (either the closest point or contains query), and a number of random query trials to run. The programs will time how long it takes to construct the geometric model (preprocessing time) and how long it takes to compute all the query trials. We then used Python scripts to calculate benchmarking statistics for different .obj files, query types, and trial runs. These statistics were plotted using various double bar graphs to help visualize patterns and directly compare each library's preprocessing and query times. Early tests suggest that the FCPW library is more efficient for a larger number of trial runs and is less error-prone than its existing counterpart. However, through more in-depth testing and analysis, we will be able to determine whether the FCPW library will be optimal for Zeno's next implementation.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Mikhail Krepets
Academic Institution:	Montgomery College
Major:	Computer Science
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	I plan to pursue my BS and likely also my MS in Computer Science with a focus on AI/ML at UMD, then do my best to start working full-time for NIST or NASA. I am considering also going for a PhD
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Division 771, Mathematical Analysis and Modeling Group
NIST Research Advisor:	Professor Michael Mascagni
Title of Talk:	Creating an Algorithm for Searching RNGs to Link with Test Results

Abstract:

Random number generators (RNGs) are often used in many aspects of everyday life from simulation and decision making to video games and other recreational activities. For a category of objects used so often, there must be a reliable method to test the quality of individual objects in that category. One of the most popular methods to test RNGs today is through a software library known as TestU01. Unfortunately, despite being effective at testing the quality of RNGs, TestU01 is expensive to run with the biggest test battery, BigCrush, consistently taking multiple CPU hours to test one RNG, which will inevitably take more wallclock hours. The original task was to research and figure out how to store RNGs and their TestU01 test results in a database such that they would be searchable, but figuring out a working algorithm to make said RNGs easily searchable ended up being so big that it turned into a project of its own.

Initially, a lot of time was spent on reading about RNGs and experimenting with the TestU01 software library in order to gain an understanding of TestU01 and the relevant RNGs. While becoming acquainted with them, we were also thinking of ideas as to how we could classify RNGs such that they would be searchable. Many potential algorithms were thought of, but the algorithm eventually proposed contains features from multiple of the potential algorithms we came up with along the way. It ended up being complicated to explain, but it should be relatively easy to use. This algorithm will likely be used in the database that the original project idea was supposed to create. However, it will also be usable in other contexts as long as they involve TestU01.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Ivy Liang

Academic Institution: Harvard University **Major:** Computer Science

Academic Standing (Sept. 2022): Sophomore

Future Plans (School/Career): Graduate School and Research

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

NIST Research Advisor: Peter Bajcsy and Mylene Simon

Title of Talk: Interactive Online Histogram-Based Visualization of AI Model Fingerprints

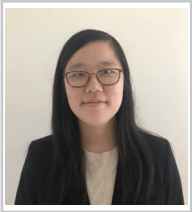
Abstract:

Previously, NIST has generated hundreds of thousands of artificial intelligence (AI) models for the TrojAI Challenge focused on detecting poisoned (trojaned) AI models. The main motivation for this project is to support discoveries/analyses of relationships between various clean and poisoned AI models by measuring their model utilization and relating it to Trojan characteristics.

In order to draw connections between AI models, the problem lies in creating interactive and traceable histograms that allow researchers to group AI models according to their characteristics, select pairs of AI models to perform qualitative/quantitative comparisons, share and discuss AI model comparisons remotely. Challenges include: interactivity over thousands of data points, traceability of histogram contributing points (AI utilization fingerprints) to their training images, and reusability of existing libraries and of the visualization prototype.

Our approach is based on the D3 JavaScript Library and Papa Parse CSV parser followed by the design of interactive, traceable, and reusable histograms. Histograms are dynamically created based on AI model attributes, including architecture name, predicted classes, Trojan triggers, and measurement probes. By selecting two contributing data points to a histogram bin, a side-by-side comparison of two AI model utilization fingerprints is enabled to quantify AI model similarities.

The resulting visualization presents a histogram of AI model utilization fingerprints with drop-down menus to allow users to select attributes for binning. Interactive images in histogram bins can be selected, new comparisons of utilization values are rendered, and buttons can trigger computations of distribution statistics.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Jane Liu		
Academic Institution:	University of Illinois Urbana-Champaign	**Major:** Computer Science
Academic Standing (Sept. 2022):	Sophomore	
Future Plans (School/Career):	Finish undergraduate	
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Information Systems Group	
NIST Research Advisor:	Timothy J. Blattner	
Title of Talk:	Implementing Real Time Constraints in Hedgehog API	

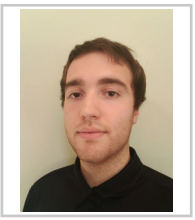
Abstract:

An operating system (OS) is system software. Among its various capabilities, the OS can manage multiple threads and rapidly switch between their executions. A real time operating system (RTOS) provides more fine grained control over multithread behavior, allowing for a deterministic response and guaranteed execution time. For example, threads with higher priority values in RTOS would be guaranteed to run over threads with lower priorities.

The ability for RTOS to provide guaranteed real-time responses is significant especially for jobs needing consistent responses within a time constraint, such as monitoring a metal additive manufacturing process in real time by keeping up with data collected from a high-speed camera.

Over the past several years, NIST has been developing a C++ library called Hedgehog, which creates task graphs for algorithms to obtain performance across CPUs and multiple co-processors. The library relies on the OS to schedule its threads and provides no real time guarantees.

The focus of this research is to extend Hedgehog to provide access to real time priorities and scheduling algorithms, so that applications utilizing Hedgehog can be more deterministic when launched on an RTOS. In this presentation, we will present the implementation efforts to add the real time capabilities into Hedgehog, and the associated performance costs. To evaluate the performance, we have implemented two algorithms; (1) the Hadamard product and (2) Matrix multiplication. We will explore the performance behaviors with and without real time constraints of these algorithms by varying priorities and thread configurations within the algorithms.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Miguel Lopez

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

Academic Standing (Sept. 2022): Senior

Future Plans (School/Career): Pursue a career in the continuously evolving field of cybersecurity

NIST Laboratory, Division, and Group: Information Technology Lab, Applied and Computational Mathematics Division, 771.02

NIST Research Advisor: Howard Cohl, Ph.D.

Title of Talk: Translating Mathematica Source Code to a Presentable LaTeX Format

Abstract:

Mathematica is a powerful programming language that is often used to handle and process mathematical data and equations. Mathematica is powered by the Wolfram Language, enabling it to define, display, and calculate essentially any level of mathematics, namely hypergeometric series in this use case. While Mathematica is well suited to manipulating, defining, and calculating these series, it is often very difficult to read and present longer equations. Through utilizing the programming language Perl, string analysis, regular expressions, and the Wolfram Engine, provided Mathematica source code is translated into the markup language LaTeX. The result is a much more user-friendly and discernible view of the hypergeometric series and other expressions contained within, and the ability to export these results easily. Translating Mathematica source into LaTeX allows for the intense computational power of Mathematica to be combined with the compatibility and readability provided by LaTeX to display the results.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Johannes Losert
Academic Institution:	Columbia University
Major:	Computer Science
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	I plan to attend graduate school
NIST Laboratory, Division, and Group:	Information Technology Lab, Software and Systems Division, Information Systems Group
NIST Research Advisor:	Derek Juba
Title of Talk:	Scientific Reproducibility of AI Trojan Detector Results

Abstract:

AI Trojans are malicious and intentional attacks that change the behavior of an AI by inserting hidden classes. To motivate research into Trojan detectors, NIST administered the TrojAI competition, where teams submit algorithms that detect Trojan AI models. The detector algorithms are known to output slightly different results across systems. These differences are problematic for scientific study of the algorithms because it means that results aren't reproducible. This problem was the motivation for my NIST SURF project in which my mentor, Derek Juba, and I researched how algorithms submitted to the TrojAI competition behave when run in different environments. Submitted algorithms are containerized using Singularity which allows them to be easily run on broad range of machines. We tried to test the algorithms on as many combinations of software and hardware as possible (CPU core count, GPU drivers, etc.) in order to deduce potential causes of differing results.

We theorized that one of the main reasons for differences in the results across systems was changes in the orders in which floating point arithmetic operations were being performed. With this in mind, we attempted to quantify the uncertainty resulting from the choice of system without running the container on different systems. We simulated different orders of operations by tweaking the weights and biases of an AI model by a small amount. We used multiple random samples of such tweaks to find the variance we can expect in results if someone were to run an algorithm on a given model across different machines. Early analysis of the data suggests that results produced on other machines agreed with the variance we predicted with our tweaks and that the statistical distributions of tweaked models are largely reproducible across machines. Additionally, we propose that that the variance of the tweaked distributions can be used to score the confidence of detector algorithms.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

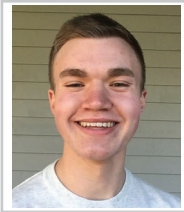
Name: Abishay Reddy

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

Academic Standing (Sept. 2022):	3.2
Future Plans (School/Career):	Pursue a Masters Degree then work in Artificial Intelligence.
NIST Laboratory, Division, and Group:	ITL, Software and Systems Division, Cyber Infrastructure Group
NIST Research Advisor:	Dr.Ram D. Sriram
Title of Talk:	Multimodal Fusion with Modality-Specific Factors for IEMOCAP dataset

Abstract:

In the scope of human-computer interaction, technology that can quickly analyze and identify emotion from varying data sources, is a coveted development. Potential applications of emotion recognition span from healthcare to gaming, only increasing demand for methods with efficient analysis and identification. Humans convey emotion through various mediums, most common of which are speech, facial expression, body language, etc. Emotion recognition technology frameworks are built upon foundational fusion methods, which synthesize various data modalities into features, utilized by prediction algorithms. This work mainly focuses on processing speech, text, and video data, and extracting the features from multiple modalities to develop a fusion model for emotion recognition tasks. We consider the IEMOCAP benchmark dataset by the processing of spliced data from modalities which includes features from audio data, video data, and embeddings from text data. These three modalities were processed for multimodal representations to recognize human emotions.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Samuel Rennich

Academic Institution: Howard Community College | **Major:** Computer Science

Academic Standing (Sept. 2022): Junior Year of Undergraduate Career

Future Plans (School/Career): Attending the University of Maryland, College Park to finish my B.S. Computer Science and earn a minor in Agronomy. Plan to work in the agricultural modeling industry.

NIST Laboratory, Division, and Group: Information Technology Laboratory, Information Access Division, Retrieval Group

NIST Research Advisor: Dr. George Awad

Title of Talk: Making TRECVID Results More Accessible and Coherent

Abstract:

NIST has run the TREC Video Retrieval Evaluation (TRECVID) program since 2001, allowing institutions to evaluate how successful their systems are at retrieving video content from textual queries. As the results of these evaluations were simply sent back to the submitting institution(s), discussed at the annual TRECVID workshop, and only reported in published papers, there was no another means for teams or the public to examine the results. The website also enables the displaying of data in more organized and visually appealing ways, such as playing the video results, corresponding to the tested queries, based on different result conditions across participating teams.

The data from these evaluations was also stored locally, with minimal organization, making it difficult to perform many statistical analyses. Building a comprehensive web interface with a suitable relational database to house the TRECVID result information was the clear solution to the problem. By developing an easy-to-use website, the information not only becomes more easily accessible to participating institutions, but it allows them to compare their tools across like systems, and over time. The website was developed with a focus on simplicity and maintainability, while also striving to remain lightweight. All data is displayed in simple tables, with a user interface that allows for easy navigation and finding of important data points with visualized results.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Vaibhav Sanjay
Academic Institution:	University of Maryland, College Park
Major:	Computer Science and Mathematics
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Graduate School/PhD
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Cyber Infrastructure Group
NIST Research Advisor:	Jacob Collard
Title of Talk:	Term and Relation Extraction in Mathematical Texts

Abstract:

There exist a variety of Natural Language Processing tools for term and relation extraction. Examples include Parmenides, a framework that applies structured and normalized terms to represent natural language, as well as DyGIE++, a deep learning system for entity and relation extraction. However, while these tools may be effective in extracting terms from scientific texts, their performance is less substantial with mathematical texts.

The two tools have previously been tested on their ability to extract terms from a collection of abstracts in the Theory and Application of Categories (TAC) journal. Parmenides extracted many valid mathematical terms, however it also extracted several times as many non-term phrases. We now hypothesize that term candidates that are part of relations, that is, subject-verb-object patterns, are more likely to be terms. Thus, a filter that removes words that cannot be found in relations reduces false-positives generated by the Parmenides term extractor.

In the case of DyGIE++, the model was retrained on TAC abstracts using author provided keywords as training data. Since the model was trained on more domain specific text, it performed stronger than the default model.

These measures increased the precision and recall of both tools by a noticable margin. In future research, we will utilize this term extraction for the creation of comprehensive knowledge graphs for mathematical domains. Further, the relations extracted by Parmenides and DyGIE++ can be employed for the evaluation of these knowledge graphs.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Yuvan Sundrani

Academic Institution: University of Maryland, College Park

Major: Information and Computer Science

Academic Standing (Sept. 2022): Junior

Future Plans (School/Career):
Pursuing a Masters degree in AI/ML or Blockchain technology while continuing to grow and expand my personal app company, Soshi.

NIST Laboratory, Division, and Group: ITL, Software and Systems Division 775.02, Information System Group

NIST Research Advisor: Antonio Cardone , Marcin Kociolek

Title of Talk: Artificial Intelligence-based texture analysis

Abstract:

Texture analysis is ubiquitous, and it finds application in both biomedical and nanomaterial research. The ability to address it in an automated fashion is greatly beneficial. However, in most cases, visual analysis and custom-tailored approaches are employed. Convolutional neural networks (CNNs) represent a viable approach to characterize image texture accurately, and in particular properties that humans can detect: directionality and granularity.

NIST researchers have been addressing AI-controlled texture analysis for years, however, they have only used synthetic data to train Artificial intelligence, not real-life data. To further advance the CNNs and our AI as a whole, we need to change the testing data to real-life images. The only barrier is that there is no efficient software allowing users to annotate real-life images to be then used for testing.

Another contribution of the GUI I created is associated with a step forward my NIST mentors are envisioning on this project. Basically, the software will enable the creation of a public database of annotated texture images that will be globally available to other scientists. Images annotated using our software will be uploaded to a public database where others can view, source, and use it. To the best of our knowledge, there is no global database that contains this information.

This would not only help researchers around the world train AIs but help advance machine learning texture analysis as a whole.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Kyle Truong		
Academic Institution:	University of Maryland, College Park	**Major:** Computer Engineering
Academic Standing (Sept. 2022):	Senior	
Future Plans (School/Career):	Career in Software Engineering	
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied Cybersecurity Division, National Initiative for Cybersecurity Education	
NIST Research Advisor:	Danielle Santos	
Title of Talk:	Evaluating the Implementation of NIST SP 800-181 in Cybersecurity-Related Job Descriptions	

Abstract:

With technology and data science becoming so prominent in society, it's becoming increasingly imperative that companies and organizations protect themselves from malicious cybersecurity threats. However, in the United States alone, there are over 700,000 unfilled cybersecurity positions. The National Initiative for Cybersecurity Education (NICE) created the NICE Framework (NIST SP 800-181) to provide a set of building blocks for describing the tasks, knowledge, and skills that are needed to perform cybersecurity work. Through these building blocks, the NICE Framework enables organizations to develop their workforces, and helps learners to engage in appropriate learning activities to develop their knowledge and skills.

The purpose of this research is to evaluate if employers are using this framework by examining job descriptions found on online hiring platforms and measuring the extent of their alignment to the Framework. The results of this research will provide insight into whether or not actions need to be taken to increase industry awareness of the Framework or to modify the Framework to better apply to employer needs.

Two methodologies will be explored to complete this project. In the first methodology, job descriptions from multiple hiring platforms such as LinkedIn and USAJobs will be graded using a rubric to determine how well they align with the framework. A job description which matches a larger amount of key words found in the knowledge, skills and tasks of a work role will score higher on the rubric. In the second methodology matching keywords and qualifications will first be found between job descriptions. After compiling a list of the most common keywords and qualifications, this list will then be compared to the Framework work role to determine how well the Framework covers what employers desire.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Ayush Varshney

Academic Institution: California Institute of Technology | **Major:** Computer Science

Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Pursue graduate studies in a field of quantum science
NIST Laboratory, Division, and Group:	Information Technology, Applied and Computational Math, Computing and Communications Theory
NIST Research Advisor:	Dr. Thomas Gerrits
Title of Talk:	Optimizing Data Communication for Low Latency Quantum Network Metrology

Abstract:

Quantum networks currently require various in-situ measurements from their components to ensure good network fidelity. Communications between quantum network nodes are carried out with single photons through the use of single-photon sources and single-photon detectors. One undesirable characteristic of these photon transmissions is substantial timing jitter associated with the single-photon detection process. To monitor this issue, each photon's emission time and absorption time is recorded with picosecond accuracy and sent to the quantum network's management system for analysis. This time-data transfer can become a considerable bottleneck in the network due to bandwidth limitations in classical data communication. Thus, we seek to reduce network overhead and optimally compress this data. In our investigation, we tested several lossless compression methods such as delta encoding, different types of variable length quantity encoding, and a hybrid approach on a sample of such data. We found that the hybrid approach produced the best results by compressing the data by 83.11% (a 5.92 compression ratio). Implementing this compression technique into quantum network metrology toolsets could significantly speed up quantum network analysis and allow for more data to be analyzed as well.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Joshua Zarb

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

Academic Standing (Sept. 2022): Senior

Future Plans (School/Career): Become a Software Engineer after receiving my bachelor's degree

NIST Laboratory, Division, and Group: Information Technology Laboratory

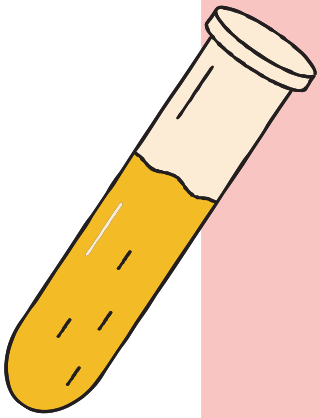
NIST Research Advisor: Dr. Ian Soboroff

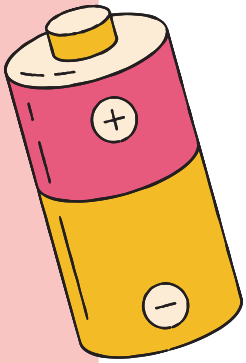
Title of Talk: Understanding Neural Search Algorithms

Abstract:

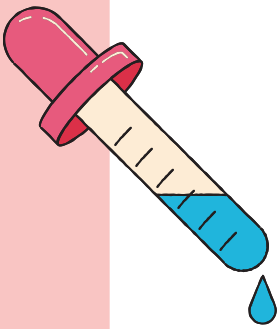
Search engines have models for predicting if a document is relevant to a query. Furthermore, in search engines, deep learning methods for predicting relevance are an emerging area of research. To determine if a document is relevant or not based on a query, search engines may use three different models. The first model is manual (non-automatic) where there is human intervention to determine whether a document is relevant or not. The next two models are considered automatic in that the query is created from the textual description of the user information needed. The first automatic model is traditional where it looks at how often terms appear in documents and uses formulas to calculate its relevance. The second automatic model is neural where neural networks are used to determine the document's relevance. The question then becomes how do all these three models compare with one another?

To answer this question, we use a query-by-query analysis approach by examining traditional, neural, and manual outputs on lots of search queries, then trying to identify patterns of success and failure for each model. I then conducted a qualitative analysis of traditional, neural, and manual ranking methods to understand the differences.





NIST | MATERIAL MEASUREMENT LABORATORY



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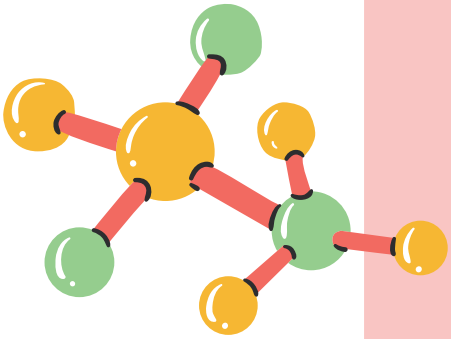
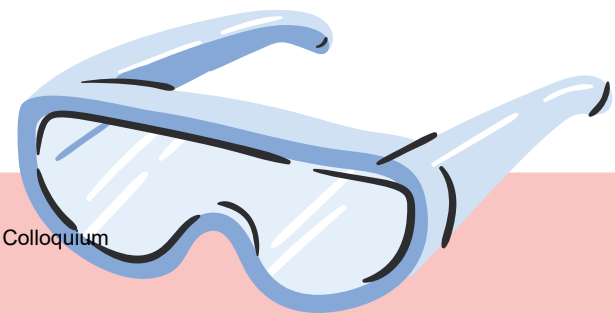




Summer Undergraduate Research Fellowship (SURF) - 2022 Participants

Material Measurement Laboratory (MML)

Marquesa Calderon

Brooke Calvo

Charlotte Dohne

Caressia Edwards

Nitin Elavarasu

Grace Finch

Melissa A. Flores-Rivera

Emily Frashure

Ross Gunther

Maggie Hampson

Aidan Knab

Bintou Koroma

Jennifer Li

Richard Ma

Jacqueline Maloney

Leilani Meyers

Terence Murphy

Yemi (Christine) Ogunsula

Ryan Puthumana

Hrishikesh Ram

Alexandra Terres

Dennis Zhao

SURF Student Colloquium

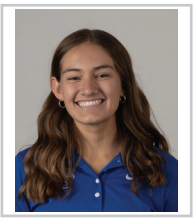
NIST – Gaithersburg, MD

August 2-4, 2022

Name: Marquesa Calderon	
Academic Institution: Hawai'i Pacific University	**Major:** Environmental Science
Academic Standing (Sept. 2022):	Junior/3rd Year
Future Plans (School/Career):	To pursue a Master's degree in Environmental Science, conduct research in Antarctica
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Biochemical and Exposure Science Group
NIST Research Advisor:	Dr. Katherine Shaw
Title of Talk:	Analysis of existing NIST SRM for microplastics

Abstract:

Microplastic research continues to grow in both its impact on and increasing ubiquity in the environment. However, there is no current standard method for the extraction of microplastics from the matrices in which they exist. This creates the need for a reference material with certified microplastic values to standardize methods. The existing National Institute of Standards and Technology Standard Reference Material 2782 Industrial Sludge (SRM 2782) was split into three subsamples and evaluated for microplastics. SRM 2782 was collected from an industrial pharmaceutical research site in northern New Jersey and has been certified to contain inorganic constituents such as silver and aluminum. This study will determine if the SRM 2782 certificate can be updated to include microplastic concentrations. It was predicted that there would be consistent concentrations of microplastics in all three replicates since they were from the same well mixed bottle homogenized in a controlled NIST laboratory. A novel density separation device (DSD) was used to extract microplastics from the sludge. Separated materials were then analyzed on a Thermo Scientific iN10 MX microFTIR. The produced IR spectra were compared against libraries of known materials to identify each particle. Ten plastic particles were identified in replicate 1 (n = 6357 particles). The most prominent polymer found in replicate 1 was nylon. However, nylon is easily mistaken for natural polyamide because they have a very similar spectra, and the majority of nylon in this sample is likely natural polyamide. Data from other subsamples will be presented. This study is a critical step toward the establishment of standard materials to test microplastic extraction methods.



SURF Student Colloquium

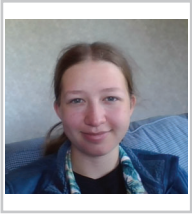
NIST – Boulder, CO
August 2-4, 2022

Name: Brooke Calvo		
Academic Institution: University of Memphis	**Major:** Mechanical Engineering	
Academic Standing (Sept. 2022):	Senior	
Future Plans (School/Career):	I plan to complete my BSME degree and potentially attend graduate school.	
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Applied Chemicals and Materials Division	
NIST Research Advisor:	Enrico Lucon and May Martin	
Title of Talk:	Assessment of Shear Fracture Appearance in Charpy Specimens of Modern Steels	

Abstract:

The Charpy test is a method used to characterize the impact toughness of materials. The instrumented version of the test uses strain gauges applied to the striker to measure applied forces. The Charpy test has been standardized by the American Society for Testing and Materials (ASTM) and the International Organization for Standardization (ISO). The standards (ASTM E2298 and ISO 14556) include four empirical correlations to estimate the shear fracture appearance (SFA, ductile portion of the fracture surface) based on the instrumented force data.

Many steels exhibit a ductile-to-brittle transition as the test temperature decreases. Within this range, both ductile and brittle features are present on the fracture surface. In this project, we analyzed data from four steels with significantly different properties to determine the SFA. This analysis is usually done optically, however for modern steels this method is often difficult to apply. We performed instrumented Charpy tests on 4340, A302B, F82H, and X52 steels at temperatures ranging from fully ductile to fully brittle behavior. The force-displacement curves were analyzed using NIST Instrumented Charpy Analysis Software (NICAS). We took photos and estimated SFA optically. Scanning Electron Microscopy (SEM) was utilized to get higher magnification images to determine the SFA more precisely. All the analyses were performed independently by an experienced user and a novice user. Regardless of experience, the results were similar across most specimens. We will compare SFA estimates from optical methods and those obtained from instrumented Charpy data to the SEM results to determine which of the published empirical correlations is more appropriate for the investigated steels.



SURF Student Colloquium

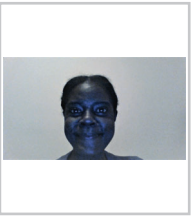
NIST – Gaithersburg, MD

August 2-4, 2022

Name: Charlotte Dohne		
Academic Institution: University of Maryland	**Major:** Criminal Justice	
Academic Standing (Sept. 2022):	Freshman	
Future Plans (School/Career):	BS in Biology at UMD, medical school, and career as forensic pathologist.	
NIST Laboratory, Division, and Group:	Material Measurements Laboratory, Division 645, Applied Genetics Group	
NIST Research Advisor:	Becky Steffen	
Title of Talk:	Creating Reference Libraries and STRBase Topic Pages on Emerging Areas in Forensic DNA	

Abstract:

The Applied Genetics Group in the Material Measurement Laboratory has a great need for a centralized reference library and updated group website. The work completed throughout this program includes searching for, adding, and organizing references for the group's publication library using EndNote, which is a commercial reference software package used to manage references when writing articles. Many of these references are being compiled and sorted on the subject of Massively Parallel Sequencing (MPS) for a workshop at the International Society for Forensic Genetics this fall. PubMed and the group's website STRBase (https://strbase-b.nist.gov/) are the main search engines being used to find scientific articles for the library, which are then stored in EndNote. A detailed search was performed for the workshop based on various forensic search terms to find a broad range of articles to cover the September 2019 to present time frame. For example, the first general search term “forensic massively parallel sequencing” resulted in 478 articles to sort through, and when five similar search terms were added over 500 results were found. In parallel, spot checks and updates of the links and pages on STRBase have also been performed before a new version 2.0 is released in the fall. Additionally, a topic page has been created for the website about an emerging technology in the forensic field, specifically, forensic microbiome research which is the study of the individualization of a person’s microbiome by specific body sites that could be useful evidence in forensic investigations. By performing advanced literature searches in emerging areas of the DNA forensic community for the group library and adding relevant content to the STRBase website, there is more current background information and knowledge of recent advances in the field of forensic genetics.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Caressia Edwards		
Academic Institution:	Fayetteville State University	**Major:**	Chemistry-Materials Science
Academic Standing (Sept. 2022):	Recent Graduate (Spring 2022)		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials and Engineering Division, and Functional Polymers Group		
NIST Research Advisor:	Dr. Frederick R. Phelan Jr. and Dr. Lilian C. Johnson		
Title of Talk:	Atomistic Molecular Dynamics Analysis of a Model Polycarbonate/Silica Composite System		

Abstract:

Polymer composites are a polymer matrix reinforced by fiber or filler phase, and are valued because of their high strength to weight ratio as well as their stiffness. Fiber reinforced composites transfer loads from the weaker polymer phase to the more durable reinforcement phase creating a stronger combined material. Load transfer ensues at the molecular level between the polymer phase and filler phase, known as the interface and interphase, this makes them a focus of scientific study. The interface is the surface area where matrix material contact the reinforcement. Interphase is the region in the vicinity of the filler where the matrix properties are modified from bulk. The goal of this project is to use molecular dynamics (MD) calculations of a polymer composite system consisting of polycarbonate restrained between fused silica surfaces to understand the interphase properties in these materials. We used MD to characterize the properties of bulk carbonate for comparison with the composite properties. A bulk polycarbonate system of 50 chains with eight monomers per chain was created. We then equilibrated the bulk polycarbonate system at a temperature of 800 K for 10 ns using the LAMMPS MD package. We cooled the surface and bulk system at three different rates 25, 50, and 100 K/ns to study the effect of cooling rate on the glass transition temperature (Tg). These runs were used to characterize the Tg as a function of cooling rate. Results for Tg as a function of cooling rate are consistent with the values in literature for this material. We then calculated structural and dynamic properties at several temperatures for the polymer matrix for comparison with properties observed in the PC/silica system. The mean square displacement and the non-Gaussian parameter of the polymer matrix are compared at varying temperatures to study how polymer motion slows and becomes more non-Gaussian as temperature decreases. Results for the bulk system will be compared with the composite system as results become available.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Nitin Elavarasu

Academic Institution: University of Virginia

Major: Chemical Engineering

Academic Standing (Sept. 2022):	3rd year of a 4-year Program
Future Plans (School/Career):	Master's in Chemical Engineering and/or a Law Degree; hoping to enter Patent Law or some STEM + Law Field: Technical Consulting
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science Division, Microscopy and Microanalysis Research Group
NIST Research Advisor:	Dr. Donald Windover
Title of Talk:	Separation of composition from structure in Micro-X-ray fluorescence measurements

Abstract:

X-Ray Fluorescence (XRF) is a type of fluorescence spectroscopy that is advantageous for its relatively simple preparation process and non-destructive nature. Fluorescence spectroscopy is a type of elemental analysis that measurers light waves emitted by a sample after subjecting it to high-energy waves. Micro-XRF is a powerful tool especially for characterizing high-Z elemental composition, however a challenge with it is separating the fluorescence data that determines the elemental composition from the diffraction peaks that cover structural information of the compound.

Through utilization of different software analysis techniques, it was possible to distill the fluorescence data from the initial micro-XRF data file that was fed through. The initial steps of isolating the requisite energy reading information from the overall file via a reader method was the same for each process. This method categorized the data file into folders and subfolders using a data structure and then searched through the structure to determine the energy reading values. These values were then processed using different analytical methods, including averaging the lowest and highest readouts from a set of data of the same sample to eliminate noise through sampling size and breaking down single samples into energy channel ranges to specify parts as either fluorescence or diffraction information.

The averaging method best removed diffraction data but took the longest time and memory to process, whereas the single-sample approach focused on reducing noise in a specific sample but had inconsistent success with identification. Overall, it would be of interest to strike a balance with these approaches to determine minimum and maximum channel ranges that still effectively identify data with an average-sampling method. These results serve primarily as a new roadmap for further micro-XRF software analysis that can better eliminate noise from more structurally complex data samples for higher accuracy of identification going forward.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

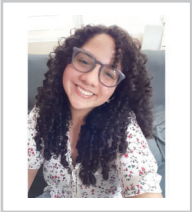
Name: Grace Finch	
Academic Institution: Virginia Tech	**Major:** Biochemistry
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	I plan on becoming a forensic chemist.
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Chemical Sciences Division, Chemical Process and Nuclear Measurements group
NIST Research Advisor:	Nicholas Sharp
Title of Talk:	Exploring Neutron Activation Analysis at the University of Maryland

Abstract:

The nuclear reactor that the National Institute of Standards and Technology (NIST) was using to run Neutron Activation Analysis (NAA) has recently gone down for repair. However, there are still routine measurements involving NAA that need to be done. The goal of this experiment was to explore the capabilities of the reactor at the University of Maryland (UMD) to perform NAA by investigating the homogeneity of the elements lanthanum, thorium, neodymium, cerium, rubidium, and uranium in three forensic glass samples. Experimentation was also done to determine whether a graphite backing matrix, or lack thereof, affects the precision of NAA measurements.

In NAA, samples are placed in polyethylene vials, which are then wrapped in aluminum foil. The wrapped foils are placed in a polyethylene container called a “rabbit,” which is irradiated in the reactor. After the vials are irradiated, they are placed on high purity germanium detectors, which acquire a gamma-ray spectrum. The gamma-ray spectrum can be used to calculate the mass fraction of the elements in the sample.

Results from the forensic glass measurement will inform the suitability of the UMD reactor for routine NAA analysis. Results from the matrix test show that the standards with no backing had greater precision than the standards with backing, which is the opposite of what was expected. This may indicate a problem with permeation of the ~5% nitric acid solution through the graphite backing. Repeating this experiment with varying volumes for both the graphite backed standard and no backing standard, and varying quantities of material for the standards with no backing may reveal why this occurred.



SURF Student Colloquium

NIST – Boulder, CO
August 2-4, 2022

Name: Melissa A. Flores-Rivera

Academic Institution: Interamerican University of Puerto Rico, San [+] **Major:** Biology

Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Pursue a Doctor of Veterinary Medicine (DVM)
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:	Structural Characterization of Extracellular Signal-Regulated Kinase 2

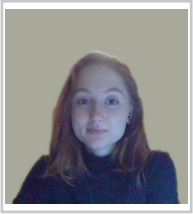
Abstract:

Extracellular Signal-Regulated Kinase 2 (ERK2) is a mitogen-activated protein kinase (MAPK) that participates in the Ras-Raf-MEK-ERK signal transduction cascade. Physiological regulation of ERK2 is important to cell growth, inflammation, proliferation, transcription, and many other cellular processes.1 The ERK signaling cascade has been implicated in many pathological conditions like cancer, arthritis, chronic inflammation, and osteoporosis.1 The cascade upstream of ERK2 may be expressed using acronyms (each K is a kinase): MAPKKKs phosphorylate MAPKKs, such as MEK, which phosphorylate MAPKs, such as ERK2. Once activated, ERK2 phosphorylates numerous cytoplasmic and nuclear substrates.2 MEK phosphorylates ERK2 at two specific threonine and tyrosine residues: T183 and Y185.3,4 The addition of the two phosphate groups activates ERK2 enabling the transfer of a phosphate group from ATP to ERK2 substrates, such as RSK1 and ELK1.3 For this summer project, the Visual Molecular Dynamics (VMD) program and MDAnalysis python scripts were used to analyze the structural features of ERK2 with and without phosphate groups, (pdbids 2erk and 5umo, respectively).3,4 We will present activation loop conformations observed in crystal structures and long conventional MD simulations carried out previously.

References:

1) Lu, N., & Malemud, C. J. (2019). Extracellular Signal-Regulated Kinase: A Regulator of Cell Growth, Inflammation, Chondrocyte and Bone Cell Receptor-Mediated Gene Expression. International Journal of Molecular Sciences, 20(15), 3792. https://doi.org/10.3390/ijms20153792

2) Fey, D., Croucher, D. R., Kolch, W., & Kholodenko, B. N. (2012). Crosstalk and Signaling Switches in Mitogen Activated Protein Kinase Cascades. Frontiers in Physiology, 3. https://doi.org/10.3389/fphys.2012.00355



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Emily Frashure
Academic Institution:	University of Maryland, College Park
Major:	Materials Science and Engineering
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Peruse a Masters Degree in Materials Science and Engineering
NIST Laboratory, Division, and Group:	MML, Materials Science and Engineering Division, Polymer and Complex Fluids Group
NIST Research Advisor:	Debra Audus
Title of Talk:	Polymer Database Pipeline for The Circular Economy

Abstract:

Currently, there is a need to improve how polymers are sorted at recycling facilities. Polyolefins, such as polypropylene and polyethylene, are some of the most common polymers. Due to insufficient sorting, when these polymers are reprocessed, there is a significant decrease in their performance and properties. However, this can be mitigated by correlating properties of recyclable polyolefins back to easy-to-take, near-infrared measurements. Doing so will thus enable improved sorting of polyolefins and allow polymers to stay within The Circular Economy. To accomplish this goal, the Community Resource for Innovation in Polymer Technology (CRIPT), an in-development platform to with the goal of increasing FAIR (Findable, Accessible, Interoperable, and Reusable) polymer data is used to make the polyolefin dataset publicly available. The platform functions by organizing, storing, and connecting data from a range of sources in a single, cloud-based database to address outstanding challenges in polymer data.

More specifically, the goal of this project was to create, using python and the CRIPT Application Programming Interface, a data pipeline starting with research data files and ending with the online database platform. The research files consist of measurement data and materials characterization information. The code splits and sorts the information, then uploads it to the corresponding nodes in the platform. These nodes connect the polymers to various property data gathered by experimentalists. By having easy-to-take measurements connected to properties measured from time-consuming, detailed experiments available to the public, recycling facilities will ultimately be able to sort the polymers with greater specificity by taking IR measurements. This would result in the reprocessed polymers being better qualified for new applications due to improved properties. These polymers would then be able to remain in use for longer, bringing the US one step closer to the goal of a circular economy.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Ross Gunther	
Academic Institution: Georgia Institute of Technology	**Major:** Materials Science and Engineering
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Materials engineering R&D work
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering, Polymers Processing
NIST Research Advisor:	Leanne Friedrich
Title of Talk:	Investigating Filament Fusion in Embedded 3D Printing

Abstract:

Embedded 3D printing is a novel approach to creating objects from soft materials. It has the potential to transform tissue engineering which uses soft materials to fabricate cartilage, vessels, tissues, and organs. 3D printing these structures with patient-specific cells would accelerate drug development, eliminate organ shortages, and reduce transplant rejection. Embedded 3D printing involves extruding a filament into a support fluid which stops soft filaments from slumping and allows creation of complex non-self-supporting shapes. While using a support expands the range of feasible printing materials, it also complicates filament fusion and print quality due to its interaction with the filament. Defects can arise at many parts of the printing process. Movement of the nozzle can deform already printed lines, filament extrusion can deform already printed lines, support material can become trapped between lines, and lines can fuse too strongly and deform into a droplet. This work investigates factors which influence these defects—namely nozzle movement, line spacing, interfacial tension, filament type, and support type. We analyze these factors by simulating numerous variations of a line printed beside or atop a second preexisting line. We use the fluid dynamics simulator OpenFOAM along with Python and ParaView to create and analyze these simulations. The findings indicate the following trends which serve as guides for others creating a printing setup. Closer line spacing increases fusion but also increases disturbance. A nonzero interfacial tension leads to smoother interfaces between lines and less trapped support. A shear thinning ink encourages less disturbance to already printed lines. Vertically-oriented lines benefit from a further spacing compared to horizontally-oriented lines. Understanding the interplay of these factors serves to improve the quality of prints and makes embedded 3D printing a more feasible method for fabrication of soft structures. This is an important step towards realizing large-scale soft material manufacturing.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Maggie Hampson
Academic Institution:	University of Maryland, College Park
Major:	Bioengineering
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Pursue a career in research and development of pharmaceuticals
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory
NIST Research Advisor:	Andrew Slifka and Matthew Connolly
Title of Talk:	Finite Element Modeling For Hydrogen Transportation & Storage

Abstract:

In a world pushing to use fewer fossil fuels, finding safe and effective renewable energy sources is crucial. Hydrogen has been looked at increasingly as a clean energy carrier. Hydrogen is gaseous and therefore it is critical that it is transported and stored safely. Few laboratories can safely test the effects of hydrogen on metals, one of these is NIST. This project focuses on developing safe transportation and storage for hydrogen so it can be used as an alternative fuel and energy carrier without the associated risks. To do this, the strength, stability, and functional lifetime of the metal used in the pipelines and pressure vessels for hydrogen must be determined. My work consists of using Autodesk inventor to replicate specific conditions similar to a laboratory setting. Through testing and finite element analysis researchers can begin to understand how hydrogen affects metals. Studies performed with Autodesk inventor don't require the waste of precious materials and researchers are kept safe from potentially hazardous conditions. Through the SURF experience, I tested various conditions, including applying an uncentered force. The first step was to develop a model for testing. The chosen model I constructed was designed to replicate specimens and test conditions used in cyclic fatigue testing. In this SURF experience, I developed and applied this model to determine the strain distribution in a specimen when a load is applied correctly and when a load is applied off-center. This can be useful for both tensile and compressive loads because off-axis loading produces different amounts of bending stresses in each case. Results are still being examined and plotting strain relative to how the load is applied will be essential to understanding the findings. The finite element analysis calculations performed during my SURF experience will help NIST researchers understand how the application of load affects the damage evolution of the specimen, and will improve the ability to run successful mechanical tests.

SURF Student Colloquium

NIST – Gaithersburg, MD

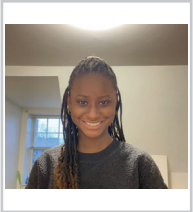
August 2-4, 2022

Name: Aidan X Knab			
Academic Institution:	University of Maryland, College Park	**Major:**	Materials Science and Engineering
Academic Standing (Sept. 2022):	3.3		
Future Plans (School/Career):	Graduate Dec 2022, Find industry job in LA		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Applied Chemicals and Materials Division, Fatigue and Fracture Group		
NIST Research Advisor:	Andrew Slifka		

Title of Talk: Machine Learning Automation of Charpy Impact Verification

Abstract:

Charpy testing is a destructive test method useful for predicting the failure of structures. Engineers using Charpy testing in accordance with ASTM E23 can have their machines indirectly verified through NIST. The MML at Boulder is designing a neural network to automate the verification of submitted images of tested samples. The neural network should determine if presented samples were tested on machines in good condition or poor condition. First, the submitted images must be prepared for training. The submitted images are cropped and stretched to all be 1000x605 pixels using a LabView program. The neural network then applies a series of convolution filters to the images before passing them through layers of nodes with activation functions. The results are compared to the correct classifications, and the error is used to reweight the paths to the nodes incrementally. This process is repeated as the error decreases. Models will be written and trained using Tensorflow with Python. The images will be duplicated and rotated slightly to enhance the dataset and avoid overfitting of the model. A dropout function that skips various nodes during training will also help reduce overfitting. Trial runs of a network designed in Perceptilabs proved successful, with ~86% accuracy. This automation will allow customers to perform an initial verification without NIST. Future models should be able to determine the nature of damage to the Charpy machines.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Bintou Koroma
Academic Institution:	University of Maryland, College Park
Major:	Bioengineering
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Graduate School/Biotech
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Polymers and Complex Fluids Group
NIST Research Advisor:	Dr. Robert Ivancic
Title of Talk:	The effect of randomness in branch spacing on LLDPE dilute solution properties

Abstract:

Today, the United States collects only 16% of plastics for recycling. Plastic recycling remains challenging because most polymers are incompatible, leading to materials with poor mechanical properties that easily break when mixed. Thus, it is essential to characterize plastic waste better to improve our ability to sort it. In this project, we attempt to improve this characterization by examining linear low-density polyethylene (LLDPE), a large and growing source of plastic waste, via a previously designed validated coarse-grained model of polyolefins in an implicit good solvent. We developed code that computes LLDPE structures with branches placed randomly along the backbone at a certain percentage analogous to industrial LLDPE. For each architecture, we used the ZENO code to calculate its radius of gyration, intrinsic viscosity, and hydrodynamic radius as functions of molecular weight and branch length . We then compared these results to previous results in which branch spacing is fixed. This comparison may facilitate future research into developing structure-property relationships for industrial LLDPE, allowing more efficient sorting of these materials in recycling streams.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Jennifer Li

Academic Institution: University of Maryland College Park | **Major:** Neuroscience and Information Science

Academic Standing (Sept. 2022): Junior

Future Plans (School/Career): I plan to pursue an MD or MD/PhD degree.

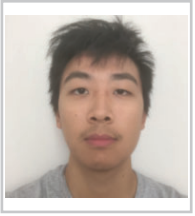
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Biomolecular Measurement Division, Bioprocess Measurements Group

NIST Research Advisor: Dr. Kurt Benkstein

Title of Talk: Characterization of Micrometer-Scale Particle Motion through Optimization of Analysis Parameters

Abstract:

Brownian motion refers to the random motion of particles suspended in a medium. Particle movement is relevant in a variety of biological and environmental applications, including the diffusion of pharmacological molecules throughout the human body. Understanding Brownian movement can improve and optimize pharmaceutical delivery to the intended area of interest. One way to elucidate particle movement is through particle tracking analysis (PTA), which provides information on the size of the particles. Particle size is related to how quickly a particle moves by Brownian motion in a medium according to the Stokes-Einstein equation. In PTA, video frames of micrometer- and sub-micrometer-scale particles of various sizes in an aqueous medium were captured using different frame rates. Initially, the expected particle movement between frames for the varied sizes and frame rates was calculated using a Rayleigh probability distribution. Next, the videos were analyzed using an image analysis particle tracker to filter particles from background noise and track their position over time. A second analysis of each particle's motion was completed using custom and open-source software developed through Python to account for frame rate and track length differences. Preliminary results on all particle sizes indicate that higher frame rates generally produce average particle size values with lower standard deviations and relative errors. Furthermore, the analyses highlight the importance of optimizing relevant video analysis parameters, including jump distance, quality threshold, track count, and track length in producing more diameters with lower relative errors. These results demonstrate the significant effects of parameter adjustments and highlight the need for parameter optimization in particle tracking methodology for estimating particle size and movement.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Richard Ma			
Academic Institution:	UC Berkeley	**Major:**	Materials Science and Engineering
Academic Standing (Sept. 2022):	Senior		
Future Plans (School/Career):	Pursue PhD		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group		
NIST Research Advisor:	Brian DeCost, Howie Joress		
Title of Talk:	Improving robustness of active learning to accelerate XRD measurements of metal alloys using NMF		

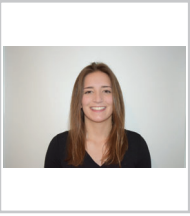
Abstract:

X-ray diffraction (XRD) is a powerful analytical technique that allows complex insight into a material's structural properties. Such experiments can be very time-consuming. When mapping complex samples, such as a composition spread thin-film requiring tens to hundreds of measurements, experimentation can take several days. Our objective is to improve mapping efficiency by applying active learning techniques to reduce the number of points to be measured while still maintaining near-complete knowledge of the sample. This is achieved by using previous knowledge to intelligently select which points to sample.

First we perform non-negative matrix factorization (NMF) on the existing XRD dataset, decomposing it into a set of constitutive basis patterns and weights which when multiplied approximate the original data. Nominally, each basis pattern should correspond to a distinct phase in the material. Peak detection algorithms are then used to detect and log the peaks in each basis pattern.

The peaks from the basis pattern are used to initialize and constrain least squares fits to the data, serving as reference points to observe changes between patterns and allowing individual patterns to be fitted using knowledge informed from the entire dataset. Fitting the data with a set of pseudo-voigt peak profiles and a background polynomial, a parameterized peak list (parameters including peak intensity, amplitude, location, etc) may be obtained for each pattern. In this manner, peaks can be tracked as they shift and broaden, and can be identified with context even when they are locally/individually difficult to distinguish from the background.

Once modeled, a set of mathematical relationships, such as a Gaussian process, may be established between the sample coordinates and the parameters of the measured peaks. By applying these methods, these relationships can be leveraged during data collection to intelligently select which points to sample, reducing knowledge-poor measurements.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Jacqueline Maloney

Academic Institution: SUNY Geneseo | **Major:** Biochemistry

Academic Standing (Sept. 2022): College Senior

Future Plans (School/Career): Graduate or medical school to obtain my doctorate

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Office of Data and Informatics, Group 0

NIST Research Advisor: Dr. June Lau

Title of Talk: Evaluation of the Microscopy NexusLIMS Search Functionalities

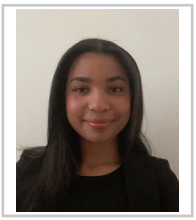
Abstract:

NexusLIMS is a laboratory information management system that curates and manages electron microscopy session data at NIST. NexusLIMS strives to maintain data that is consistent with the FAIR data principle1. It is also tool for researchers to search, explore, and download data their data through a web interface powered by NIST's configurable data curation system (CDCS).

The emphasis of this work centers around human and machine discoverability of data already residing in the NexusLIMS database. Some context: In any scientific discipline (e.g. electron microscopy), the research community often uses different words and phrases with similar meanings interchangeably. Although the researcher themselves know and understand the relationships among similar terms, this knowledge is not machine actionable (i.e., when a search is performed) until those relationships are explicitly defined for the machine.

Previously, this project had developed an electron microscopy thesaurus of commonly use terms and their relationships represented as a similarity score, using natural language processing. My work consists of the implementation of this thesaurus into the three different search modalities supported by CDCS: elastic search, search operator, and auto complete. Auto complete is a whole-word-based function that generates search options as you type in the search bar. The search operator functionality allows the user to filter their search results based on the specific operator in use. Elastic search enables one to search large volumes of data quickly by searching an index instead of text directly. We hope to demonstrate how these search modalities differ and can improve the search quality from both the human and the machine perspective.

1. Jansen, Mascha. “Fair Principles.” GO FAIR, 21 Jan. 2022, https://www.go-fair.org/fair-principles/.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Leilani Meyers

Academic Institution: Boston University | **Major:** Biochemistry and Molecular Biology

Academic Standing (Sept. 2022): Junior

Future Plans (School/Career): Attend dental school

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Biomolecular Measurement Divison

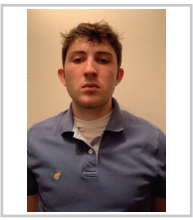
NIST Research Advisor: Dr. Tytus Mak

Title of Talk: Assessing Ambiguities in Metabolite Identification when Analyzed by LC-MS/MS

Abstract:

Liquid chromatography-mass spectrometry (LC-MS/MS) is a technique that pairs the chromatographic separation of a biological sample with an analytical tool that elucidates information on the molecular weight and abundance of its contents by ionizing the molecular components, resulting in a retention time, relative abundance, and mass-to-charge (m/z) ratio value for each analyte in the sample. This method is used for metabolomics, the comprehensive study of the small molecules involved in metabolism, because it allows the composition of large quantities of diverse and complex biological samples to be determined efficiently without extensive preparation. Metabolomics allows biological pathways to be evaluated to study biochemical mechanisms and to further understand diseases.

A major challenge encountered when using LC-MS/MS is the ambiguous identifications of compounds. In this work, a program was created to facilitate the analysis of metabolites with uncertain identities. To highlight ambiguities, a CSV parser was written in Python to isolate data from CHO cell metabolite extract samples with duplicate identifications (facilitated by matching InChIKeys). The adduct type and retention times of these compounds were displayed for comparison. A dot-product-based score (ranging from 0 to 999) is assigned for each library match, with higher scores indicating a better match to the library's reference spectrum. Analytes with a second hit having a score within 50 points were flagged as ambiguous to be further studied using MetaboPique and MetaboVision, where users can visually examine extracted ion chromatograms associated with each analyte and inspect MS2 spectra. This work helps to improve compound identification confidence and highlights the importance of discretion when interpreting hits by revealing data ambiguity. The program located many ambiguities throughout the data, showing up to nine duplicates of a certain analyte. The cause of these ambiguities can be further studied to understand how they can be reduced to maximize identification certainty.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Terence Murphy
Academic Institution:	Purdue University
Major:	Computer Engineering
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	R&D in the field of computer engineering.
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Biosystems and Biomaterials Division, Cellular Engineering Group
NIST Research Advisor:	Samuel Schaffter
Title of Talk:	A Versatile Simulator for Cotranscriptionally Encoded RNA Strand Displacement Circuits

Abstract:

Cotranscriptionally encoded RNA strand displacement (ctRSD) circuits are an emerging technology for programmable and scalable molecular computations. ctRSD circuits can execute multilayer cascades, logic, and signal amplification, and these elementary functions can be integrated to orchestrate sophisticated information processing tasks like digital calculations and pattern recognition. To design, predict, and understand the behavior of ctRSD circuits, a theoretical model that describes the kinetics of a broad range of possible reactions is needed. A user-friendly, scalable simulator that encompasses all conceivable ctRSD reactions with arbitrary circuit connectivity would fill this need and could be used to prototype new designs and compare experiments to theory. Here we develop a comprehensive kinetic simulator written in Python. We first derived the mass action differential rate equations that describe how the ctRSD species change with time for any combination of 40+ possible reactions. These equations are then numerically integrated in Python to simulate the kinetics of a given system. Instead of creating specific rate equations for each simulation, we implemented the equations with matrix algebra. This allows ctRSD components to be connected in any arbitrary way, and linear algebra populates the various matrices based on the components specified by the user so that one set of governing equations encompasses all possible systems. Lastly, we developed an intuitive user interface that enables straightforward definition of custom parameters. We validated the simulator with 50+ detailed examples spanning all possible reactions. A current limitation is the time required to simulate systems involving reactions at very different time scales. Future work could address this issue by integrating our simulator's front end to alternative solvers, such as BioGenNet and Bioscrape, that handle disparate timescales. To aid experimentalists in prototyping ctRSD circuits and facilitate the broader adoption of this technology, we have launched a website with in-depth simulator instructions and examples.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Christine "Yemi" Ogunsola

Academic Institution: Montgomery College | **Major:** Chemical and Biomolecular Engineering

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): I plan to continue my education into graduate school to gain a job combining AI and natural Sciences.

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Materials Measurement Science Division, Surface & Trace Chemical Analysis Group

NIST Research Advisor: Dr. Edward Sisco and Dr. Arun Moorthy

Title of Talk: Building and Expanding the Drug DART-MS Forensics Database with Automated Tools

Abstract:

With the ability to create a new drug with simple modifications during its synthesis, identifying illegal drugs has become increasingly challenging. At NIST, we research new tools such as Direct Analysis in Real-Time Mass Spectrometry (DART-MS) that forensic scientists can use to get rapid and more accurate data than traditional instrumentation. Hence, the NIST DART-MS Forensics Database, which contains mass spectra of various drugs and can help assist forensic laboratories in drug identification, was created.

Building a mass spectral database is a complex and financially expensive process. Due to time and financial constraints, it is imperative that we understand what drugs are valuable and prioritize them in our database. To help identify which drugs should be included, mathematical models were created to propose optimal combinations of drugs to expand the database. These models consider and evaluate various value paradigms for optimal solutions using several algorithmic approaches.

Additionally, a database sometimes has the potential to include human and computer-generated errors. For the NIST DART-MS Forensics Database, one tool that is regularly used for identifying inconsistencies is Validation User Friendly (VUF). VUF checks the metadata of every entry in the intermediary step of the database building process. Each chemical identifier (molecular mass, canonical SMILES, InChI code, InChI key, and class) is validated against the provided chemical formula (assumed as fact). The data is verified by a custom script and compiled into a user-friendly validation application. Depending on the user's needs, the dataset can be filtered by multiple values and downloaded.

This presentation will cover these tools' automated methods for building and expanding our database, and thereby ensuring accurate and relevant information for the forensic community.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2022

Name: Ryan Puthumana

Academic Institution: University of Maryland, College Park

Major: Bioengineering

Academic Standing
(Sept. 2022): Senior

Future Plans
(School/Career): Biomedical research/industry and possible graduate school

NIST Laboratory,
Division, and Group: Material Measurement Laboratory

NIST Research
Advisor: Dr. Tyler Martin

Title of Talk: Optimization of Clustering Algorithms for Small Angle Scattering of Polymer Formulations

Abstract:
There remains a persistent need in the field of materials development to characterize the structural properties of polymer samples dissolved in oil and water solvents. Oftentimes, the amphiphilic nature of these polymer-solvent mixtures means that a variety of microstructures are formed, including micelles, lamellae and cylinders. Neutron scattering is a useful technique to characterize these structures, but the process of data analysis is time consuming and requires deep expertise. In order to develop automated analysis strategies that characterize microstructure, we examined three common clustering methods — KMeans, affinity propagation, and DBSCAN. While affinity propagation and DBSCAN automatically determine the number of clusters in a dataset, KMeans requires a secondary method for this purpose and we additionally explored three potential options: silhouette, gap-statistic, and elbow methods. We found that while the DBSCAN method had the best performance with default parameters, the affinity propagation method offered the optimal combination of simplicity and flexibility with some modification. When compared to our gold standard of manual clustering by hand, affinity propagation offered a high Fowlkes-Mallows score indicating optimal clustering. Additionally, affinity propagation contains a "preference" input term that can be modified based on data-specific knowledge for added tunability. As KMeans required a separate step to determine the optimal number of clusters it was more inefficient compared to the other algorithms. In conclusion, we have benchmarked several data clustering methods and other ancillary analyses related to the clustering of small-angle scattering data of polymer materials. This project serves to establish a relatively simple and efficient pipeline for researchers and inexperienced lay people alike to analyze small angle scattering data of soft materials.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Hrishikesh Ram

Academic Institution: North Carolina State University | **Major:** Chemical Engineering + Chemistry

Academic Standing (Sept. 2022): Rising Sophomore

Future Plans (School/Career): Graduate School in Chemical Engineering/Chemistry/Polymer Science

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

NIST Research Advisor: Jennifer A. Clark (NRC)

Title of Talk: Interaction Energies of Zwitterionic Polybetaines with NaCl

Abstract:

Polybetaines are a family of zwitterionic monomers with both positively and negatively charged groups that exhibit stimuli-responsive properties with applications in biomedicine and membrane design. The tendency of these materials to expand in response to increased salt concentration is the opposite of entirely anionic or cationic polyelectrolytes. Thus, this response to salt is termed the anti-polyelectrolyte effect, and is likely caused by competitive ionic interactions between the polyzwitterions and salts. Because such complex interactions are difficult to deconvolute with experimental methods, computational simulation (e.g., density functional theory (DFT)) will aid in understanding polybetaine interactions with salt. In an ongoing project, systems consisting of the 2-(acrylamidoethyl-dimethyl-ammonium) propyl-1-sulfonate sulfobetaine monomer interacting with NaCl in aqueous solution were probed using molecular dynamics (MD). Geometries of target ionic groups (monatomic and polymeric) were extracted from these MD trajectories to serve as input structures for DFT calculations. Water molecules within approximately 2.8Å of hydrophilic groups were included to explicitly represent the first hydration shell. Frames were then grouped into categories by anticipated interactions based on the proximity between ionic groups. Random samples were extracted for each category and input into DFT calculations. With the IEFPCM/B3LYP-D3/aug-cc-pVDZ model chemistry, the absolute solvation free energies of Na+ and Cl- are determined using the primitive quasichemical theory (pQCT) for sodium-water and chlorine-water clusters of varying coordination. The accuracy of the pQCT setup compared to experimental values for monatomic ions allows the application of the same method to sampled sulfobetaine monomer configurations. Subsequently calculating gas-phase binding energies in conjunction with solvation free energies will help quantify the free energy contributions involved in various competing ionic interactions within ion-polymer systems. Thus, this work will help characterize the competitive ionic interactions that result in the stimuli-responsive phenomena observed with polybetaines.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Alexandra Terres
Academic Institution:	University of Maryland
Major:	Materials Science and Engineering
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Plan to pursue a Masters Degree or Ph. D. in Materials Science
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Measurement Science Division, Materials Structure and Data Group
NIST Research Advisor:	Benjamin Dolata, Lawrence Friedman
Title of Talk:	COMSOL Simulations of Contact Line Propagation in Additive Manufacturing with Ceramics

Abstract:

Ceramic slurries in additive manufacturing (AM) have the potential to revolutionize biomedical, aerospace, and electrical engineering. The direct ink write (DIW) process provides a reliable way of producing custom and individualized products with slurries, capable of expanding the AM industry. One aspect of the on-going research into this process is building a better model for slurry extrusion with regards to bead shape that will allow for better control and development of DIW printing. We used COMSOL Multiphysics software to simulate the propagation of laminar single-phase flow of a non-Newtonian, Herschel Bulkley-Papanastasiou slurry through a pipe using a moving-mesh method to refine the simulation at the point where the slurry/air contact line means the pipe wall. Previous constitutive models utilizing a phase-field or level set method have been insufficient at defining this point, as the contact angle exceeds 180˚, thereby "flowing" outside the bounds of the pipe. Two conditions are integral in determining the dynamic behavior of the contact angle: the capillary number and the Navier slip boundary condition. The former describes the ratio of surface forces to viscous forces, analogous to surface tension and fluid friction; the latter is a condition applied at the wall that allows the line to move freely through the simulation. By kinematically coupling the contact line dynamics with fluid velocity and refining the mesh significantly at this point, we demonstrate that the necessary mesh refinement for a successful simulation is a function of capillary number.

SURF Student Colloquium

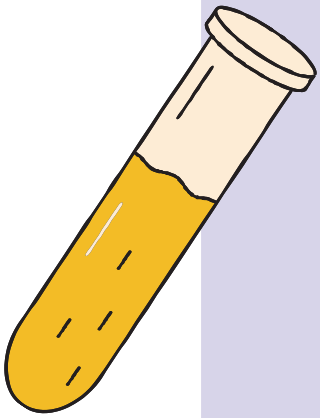
NIST – Gaithersburg, MD

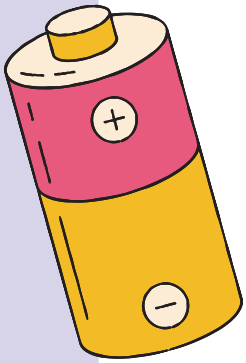
August 2-4, 2022

Name: Dennis Zhao		
Academic Institution: University of Maryland College Park	**Major:** Materials Science and Engineering	
Academic Standing (Sept. 2022):	Sophomore	
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 Ternary Phase Diagrams Using Machine Learning	

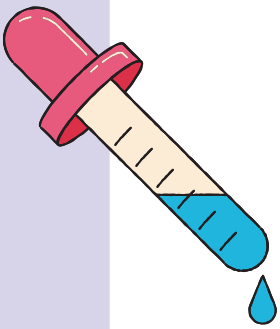
Abstract:

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'.

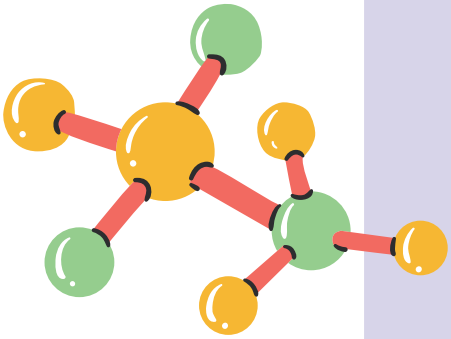


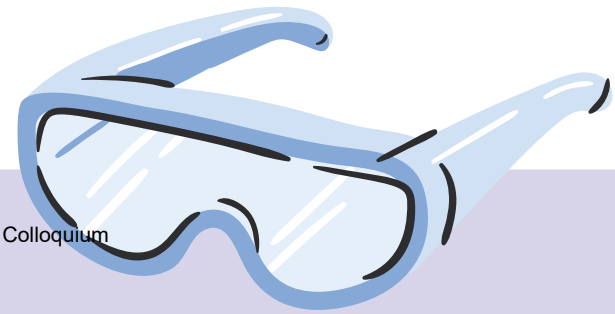


NIST | CENTER FOR NEUTRON RESEARCH



2022





Summer Undergraduate Research Fellowship (SURF) - 2022 Participants

NIST Center for Neutron Research (NCNR)

Benen Crombie

Shriya Haravu

Amy Musser

John Nunez

Jack Rooks

Christopher Stallard

Kim Taylor

Washat Ware

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Benen Crombie
Academic Institution:	University of Virginia
Major:	Mechanical Engineering
Academic Standing (Sept. 2021):	Junior
Future Plans (School/Career):	I intend to pursue a career in engineering and potentially attend a graduate progam for engineering or computer science.
NIST Laboratory, Division, and Group:	Center for Neutron Research, Reactor Engineering
NIST Research Advisor:	James Whipple
Title of Talk:	Automating the Fuel Element Visual Inspection Process at the NCNR Reactor

Abstract:

On February 3, 2021, the NCNR reactor experienced a fuel element failure resulting from an improper latching of one of the fuel elements. This caused the element to exceed its allowable temperature. This was a failure of the inspection checks that must occur before the reactor is operational, and new checks were implemented at the NCNR in response. One of these checks is a visual check of each fuel element. Reactor operators check that the latch bar of the fuel element is in line with the fuel element itself. This inspection process takes about two hours. The goal of this research project is to automate the process in a custom computer application using video and image processing techniques.

Our program is built in Python and utilizes a Computer Vision library called OpenCV. The program takes the video from the visual inspection tool camera as the input and returns a report consisting of pictures of each fuel element and their respective offset angles. Reactor operators can then view the output report to perform a final human inspection to ensure that all fuel elements are latched properly. To accomplish this we implemented contour detection, which outlines large shapes that have the same light intensity. Afterward, the next step in the project was calculating the offset angle of the latch bar. Once we found the bounding boxes of the fuel element and the fuel element latch bar, the angle was calculated.

Our program automated the inspection checks and shortened a 2 hour process to a few minutes. This program can be modified to ensure safe and efficient inspections of reactors at other facilities and save reactor operators upwards of 10 hours of manual inspections every year.

SURF Student Colloquium

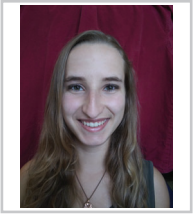
NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Shriya Haravu
Academic Institution:	UNC Chapel Hill
Major:	Astrophysics + Mathematics
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Hope to work in industry before going to graduate school
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron-Condensed Matter Science Group
NIST Research Advisor:	William Ratcliff
Title of Talk:	Automatic Identification of Regions of Neutron Diffraction Patterns Changing During Phase Transition

Abstract:

Neutron scattering is an exquisite probe of the crystal and magnetic structure of materials. Increasing the efficiency with which neutron scattering data can be taken is important because there are a limited number of neutron facilities in the world. We know from previous experiments that there exist specific regions of diffraction patterns which change with temperature upon a phase transition. These changes in the diffraction pattern can inform us about changes in the crystalline and magnetic order in the material. Our goal is to automatically identify the regions mentioned above using diffraction patterns. In this project, I work with simulated diffraction patterns and use the DREAM (DiffeRential Evolution Adaptive Metropolis) algorithm to automatically fit peaks to the data. Following this identification of peaks, we determine how individual peaks shift with temperature while also monitoring the appearance/disappearance of peaks. By measuring a diffraction pattern above and below the transition, this will allow us to determine which regions to follow during the phase transition.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Amy Musser
Academic Institution:	University of Maryland College Park
Major:	Bioengineering
Academic Standing (Sept. 2022):	Recent Graduate
Future Plans (School/Career):	Industry
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, NCNR Neutron Condensed Matter Sciences
NIST Research Advisor:	Yimin Mao
Title of Talk:	Multi-Scale Structures of Starch as Revealed by Scattering Techniques: From Unit Cell to Nanostructure

Abstract:

Starch is a form of energy storage produced by plants, abundant in seeds, roots, and tubers. As a common source of dietary calories, starch structure and crystallinity play a pivotal role in its digestion, which is an important aspect of human dietary health, gut health, and overall well-being. We examined the multiscale structures of four different starches, specifically, waxy maize, normal maize, high amylose maize, and pea starch, using wide- and small-angle x-ray scattering techniques (WAXS/SAXS). WAXS was used to probe starch crystal structures as well as the content of crystalline portion in starch granules. In addition, grain size of starch crystals can be calculated by diffraction line profile analysis. SAXS was used to characterize nanoscale structures. It was identified that starch crystals in waxy maize and normal maize are of the A type, whereas those in high amylose maize are of the B type. Pea starch possesses a unique crystal type, which is arguably considered as a mixture of type A and B. It was found that water can significantly enhance starch crystallization: after hydration, a dramatic increase of crystallinity and perfection of crystals were revealed by WAXS, and a formation of nanoscale lamellar structure consisting of amorphous and crystalline layers occurring in an alternating manner by SAXS. Our quantitative analysis can provide insights into structural roots of physical properties of starch, such as pasting and enzymatic hydrolysis efficiency. Neutron and X-ray scattering will be used to further decipher water partition in starch multi-scale structures.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

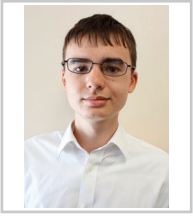
Name: John Peter J. Nunez		
Academic Institution:	Virginia Commonwealth University	**Major:** Mechanical Engineering
Academic Standing (Sept. 2022):	Junior	
Future Plans (School/Career):	Aeronautical Engineer (Government (Department of Defense)/Defense Company)	
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research	
NIST Research Advisor:	Dr. Jonathan Gaudet	
Title of Talk:	Revealing the magnetism of Weyl semimetal CeAlGe	

Abstract:

Weyl fermions are massless and highly mobile particles. They also possess a form of chirality in which their spin is either in the same direction as motion (right-handed) or in the opposite direction (left-handed). Their basic nature means that Weyl fermions move very quickly on the surface of the crystal with no backscattering, which hinders efficiency and generates heat in normal electronic materials.

Given that Weyl fermions have not yet been directly observed in nature, it has been discovered that they accurately characterize the emerging electrical properties of select crystalline semi-metallic materials that either break inversion or time-reversal symmetry. This research focuses on the semi-metallic CeAlGe material, whose crystal structure deviates from inversion symmetry to allow the emergence of Weyl fermions. Additionally, the time-reversal symmetry is broken by the Ce3+ low temperature collective magnetism, which affects the Weyl characteristics. Thus, CeAlGe offers a unique template for researching the relationship between Weyl fermions and magnetic properties.

In this presentation, we will go into the specifics of the CeAlGe compound's magnetic structure and spin-order analysis, which we conducted using neutron diffraction. We will present the single crystal neutron diffraction data we carried out to determine the CeAlGe nuclear and magnetic unit cell. We discovered that the Ce spins in the magnetic unit cell are pointing within the basal plane and have compositions that are both ferromagnetic and antiferromagnetic. Given this, since zero field neutron diffraction cannot definitively reveal the specifics of the collinear structure, we will also discuss our in-field neutron diffraction data that can be refined to resolve this uncertainty. The relationship between the magnetism and the Weyl fermions in CeAlGe will then be presented.



SURF Student Colloquium

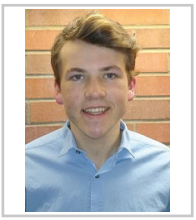
NIST – Gaithersburg, MD

August 2-4, 2022

Name: Jack Rooks	
Academic Institution: SUNY at Buffalo	**Major:** Chemical engineering
Academic Standing (Sept. 2022):	Graduated
Future Plans (School/Career):	Chemical engineering PhD program at University of Delaware
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research (NCNR), Neutron Condensed Matter Science Group
NIST Research Advisor:	Peter Gilbert
Title of Talk:	Particle orientation in soft materials from small-angle neutron scattering

Abstract:

Many soft materials, like polymers, derive their mechanical strength and flexibility from molecular and nanostructure orientation. Any particle or molecule that is longer than it is wide has orientation, and this orientation can be manipulated by an external force, such as flow, to modify orientation-dependent material properties. Small angle neutron scattering (SANS) can measure nanoscale orientation within a material, and traditional analysis yields an estimate of the average orientation angle. Particles are often imperfectly oriented in soft materials, resulting in a distribution of particle orientations about an average angle. We introduce a novel analysis method to extract the width of the orientation distribution from experimental SANS data for flow-aligned cylindrical micelles. This analysis requires data collected from different perspectives of micelle orientation. These perspectives are then assembled into a single estimate of the orientation distribution. Our analysis provides more information on the orientation distribution than previous approaches. This new orientation information will enable more precise tuning of material properties that are linked to orientation.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Christopher Stallard

Academic Institution: University of Minnesota | **Major:** Chemical Engineering

Academic Standing (Sept. 2022): Sophomore

Future Plans (School/Career): Go to graduate school, get a PhD, and work in either industry or government labs

NIST Laboratory, Division, and Group: NIST Center for Neutron Research, Neutron-Condensed Matter Science Group

NIST Research Advisor: Ryan Murphy

Title of Talk: Developing a User-Friendly Framework for Stopped Flow SANS at the NCNR

Abstract:

Small-Angle Neutron Scattering (SANS) is a technique that can measure structural properties of materials at nanometer to micrometer length scales. Recently, there have been developments in the use of time-resolved SANS to study kinetic processes and the resulting changes in small-scale structure. This technique is particularly important in the study of biological and self-assembled systems. In order to probe shorter timescales (from 100ms-10s), it is necessary to begin measurement as quickly as possible after mixing. Stopped-flow techniques mix components using a series of pumps, valves, and one or more flow-through mixer. This lowers the "dead time" between mixing and observation to <1s.

The Center for High Resolution Neutron Scattering (CHRNS) is developing a stopped-flow SANS system for routine use, in order to expand its measurement capability for facility users. As a complementary measurement technique, UV-Vis spectra are collected simultaneously with SANS measurements. In this project, I created a single program to control all the experiment hardware, including pumps, valves, pressure sensors, and the UV-Vis spectrometer. This program provides a simple way to control, monitor, and automate experiments. Using this program, I characterized the response of the UV-Vis spectrometer to various concentrations and mixing ratios of fluorescent dye/quencher pairs. Additionally, I propose a standard method for data analysis of both time-resolved neutron flux and 1D SANS data, and test that method using simulated data based on past experimental scenarios. This work sets the stage for consistent experimentation and analysis of stopped-flow SANS data at the NCNR.

SURF Student Colloquium

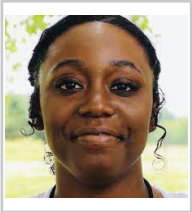
NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Kim Taylor
Academic Institution:	University of Maryland College Park
Major:	Material Science Engineering
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Completing my bachelors in Material Science Engineering at UMD and continuing on to Grad school.
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research: NCNR Neutron Condensed Matter Sciences
NIST Research Advisor:	Yimin Mao, Susana M. Teixeira, and Susan Krueger
Title of Talk:	Surfactant-Free Oil-in-Water Emulsion Stabilized by Chitin Nanocrystals: A Green Recipe

Abstract:

An emulsion is a colloidal mixture of two or more incompatible liquids, typically in a form of droplets of one phase dispersed in a matrix, such as oil droplets dispersed in their water surrounding, termed oil-in-water emulsion. The food industry is one of the most significant users of emulsion technology since many food products, such as milk, butter, and creams, need to be manufactured using multiple, incompatible liquid components. Emulsions need to be stabilized by amphiphilic species such as surfactants to prevent them from agglomerating, which often leads to environmental and health concerns. Alternatively, a new type of emulsion, Pickering emulsion, can be produced when using colloidal particles as an emulsifier. In this study, we used chitin nanocrystals (ChNCs) to produce oil-in-water Pickering emulsions, with the goal to provide a green recipe applicable to various food products. Chitin is mainly sourced from fishery wastes; it is the second most abundant biomass on the earth. We applied phosphoric-acid (PA) hydrolysis and 2,2,6,6-tetramethylpiperidine-1-oxyl(TEMPO) mediated oxidation methods to produce ChNCs (PA-ChNC and TEMPO-ChNC) with varied size and surface chemistry. Nanostructure of the rod-like ChNCs were characterized using dynamic light scattering (DLS) and small-angle X-ray scattering (SAXS). It was found that both types of ChNCs were able to form stable Pickering emulsions at an oil (medium chain triglycerides)-to-water ratio of 1:9 (volume ratio). PA-ChNC produced a smaller droplet size of ~2 microns with a relatively narrow size distribution, while TEMPO-ChNC produced droplets with a broad size distribution ranging from a few microns up to ~20 microns. On-going investigation focuses on using scattering and microscopic techniques to characterize the oil-water interface stabilized by ChNC, to correlate the ChNC characteristics to emulsion structures and properties.



SURF Student Colloquium

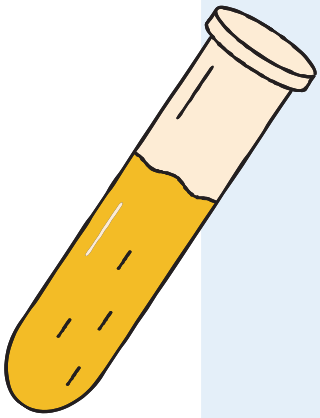
NIST – Gaithersburg, MD

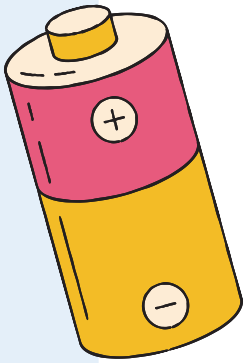
August 2-4, 2022

Name:	Washat Roxanne Ware
Academic Institution:	Fayetteville State University
Major:	Chemistry w/ conc. Materials Science
Academic Standing (Sept. 2022):	Recently Graduated
Future Plans (School/Career):	PhD in Materials Science and Engineering and eventually work in prosthetics research
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, NCNR Neutron Condensed Matter Sciences
NIST Research Advisor:	Rachel Ford
Title of Talk:	Determining the validity of Guinier analysis in slit-smeared small angle scattering data

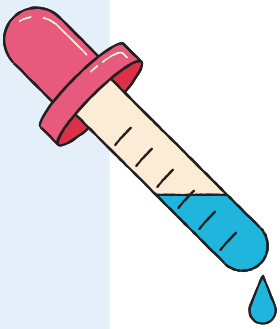
Abstract:

Small angle scattering (SAS) techniques are powerful methods for probing structure ranging from nanoscopic to mesoscopic scale. A common method for analyzing SAS data is Guinier analysis, which enables the determination of the radius of gyration, Rg, without prior knowledge of the particle morphology. Guinier analysis was developed specifically for unsmeared data. The Guinier model may work well for certain instrument smearing, namely smearing from instruments with slit geometry. Therefore, Guinier analysis is typically not used on slit-smeared data, such as data from ultra-small angle neutron scattering (USANS) instruments. We seek to determine whether the Guinier approximation holds for slit-smeared data. We apply Guinier analysis to simulated data for a variety of particle morphologies both with and without slit smearing. We report the models for which the Guinier approximation holds in slit-smeared data, as well as boundary conditions for models where slit-smearing produces a non-negligible deviation of the extracted Rg.





NIST | PHYSICAL MEASUREMENT LABORATORY



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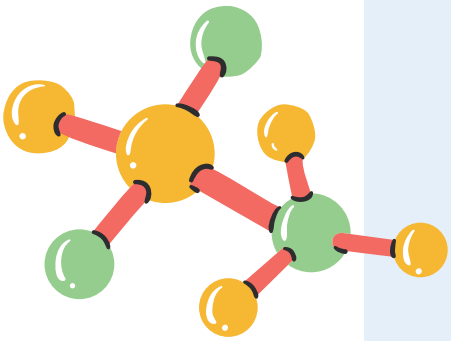


Summer Undergraduate Research Fellowship (SURF) - 2022 Participants

Physical Measurement Laboratory (PML)

Nicolas Aguilar

Max Buskirk

Briana Chen

Hayden Craun

Aagam Dalal

William Dienstfrey

Michael Gabe

Michael Gutowski

Samir Kulkarni

Connor Lewis

Gabirel Lewis

Faith Makumbi

Satvik Manjigani

Evan McClintock

Shawn Meyer

Daniel Quinter

Abrar Sheikh

Hunter Staiger

Grace Tang

Travis White

Lucy Yagodich

Joshua Young

Helen Zhang

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Nicolas Aguilar

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

Academic Standing (Sept. 2022): Senior

Future Plans (School/Career): Currently planning on obtaining a master's degree and pursuing a career in engineering

NIST Laboratory, Division, and Group: PML, Quantum Measurement Division, Mass and Force Group

NIST Research Advisor: Jon Geist

Title of Talk: Testing Calibration Uncertainty With Low Cost Inertial Measurement Units With A Pendulum Method

Abstract:

NIST serves as the primary measurement and calibration laboratory for the nation and as part of that, the Mass and Force Group within the Physical Measurements Laboratory focuses on advancing measurement technologies for inertial measurements. A big part of this includes the use of Inertial Measurement Units (IMUs), which consist of a mix of tri-axis accelerometers, gyroscopes and magnetometers. IMUs are used in a vast amount of technologies in today's era, including smartphones, vehicles, and drones as they are essential in determining the motion and position of the device.

This project focuses on testing the calibration uncertainty of the Adafruit nRF52840 Bluefruit Sense (a micro-electromechanical IMU that sends acceleration and rotational data to a device via Bluetooth) by using a calibration method that was previously developed by NIST. The first phase of this method uses gravity and the intrinsic properties of the IMU to calibrate the sensor in static conditions with a predicted uncertainty under one tenth of a percent (based on previous results done by NIST). This process is done by running the IMU under different orientations in a cube to see the offset within each accelerometer. The second phase of the method consists of using a pendulum to collect both gyroscope and accelerometer data to calibrate the gyroscope with the accelerometer data and with the effective length of the pendulum including uncertainties. We will compare the manufacturer's calibration with the calibration done on the accelerometer to see its differences and effectiveness.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Max Buskirk
Academic Institution:	California Polytechnic State University
Major:	Chemistry, Physics
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Graduate School in Physics or Chemistry; preferred topics near AMO Physics or Chemical Physics. Career involving the physical sciences somehow.
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory; Nanoscale Device Characterization Division; Advanced Electronics Group.
NIST Research Advisor:	Yaw S. Obeng
Title of Talk:	Analysis of Solder Joint Failures using Resistance Measurements

Abstract:

Solder joints found in electronic systems are susceptible to failure in two main groups: hard failures and no failures found (NFF). NFF failures are responsible for half of all failures in solder joints. The focus of this research is to detect NFF failures before complete failure. By determining how solder joints fail in NFF failures, the Department of Defense could save upwards of $2 billion annually.

Sample boards were analyzed in a thermally controlled chamber cycling between 0 °C and 100 °C, while measuring some electrical properties of the joints. Comparing cycle number, the corresponding temperature, and the microwave signal return loss yielded some previously unidentified details, including nearly abrupt jumps. These gave some insight into these NFF failures, with the jumps possibly corresponding to stages of failure of the solder joint. But, some past work suggested that these measurements detected complete failures after when they would be detected by DC resistance measurements. In this work, DC resistance measurements of the joint failure are analyzed in order to, similarly, find any previously unidentified detail. This will help further characterize solder joint failures under thermal cycling, and improve measurement techniques. Preliminary results show a lack of temperature dependence of the resistance, but some dependence on the cycle number has been found.

SURF Student Colloquium

NIST – Boulder, CO
August 2-4, 2022

Name:	Briana Chen
Academic Institution:	Purdue University
Major:	Aerospace Engineering
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Graduate school!
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Applied Physics Division, Quantum Nanophotonics Group
NIST Research Advisor:	Dr. Krister Shalm
Title of Talk:	Developing resources for understanding an enhanced randomness beacon

Abstract:

Public sources of randomness have powerful applications, widely affecting societal processes and outcomes such as lotteries, jury selections, and spot checking. Currently, NIST operates a public randomness beacon that periodically publishes pulses containing random values, creating a blockchain of randomness.

The research team I have been involved with aims to replace this current beacon with a next-generation beacon that is efficiently verifiable and incorporates better quantum randomness. However, both beacons utilize blockchains and specific protocols that are difficult to understand and implement, which discourages people from using the beacons in various applications. Because of this, the general public requires an educational resource that explains why randomness beacons are useful and how they can be used.

In this talk I will discuss an interactive web-based tutorial I created that introduces the fundamental concepts behind the new beacon's protocols to create trustworthy randomness. The tutorial also highlights how the beacon safeguards against illegitimate claims and manipulation. By learning about the inner workings of a randomness beacon, the tutorial's users will better understand how to apply public sources of randomness to their own ventures. This will ultimately make the randomness beacon more widely accessible and help it reach its full potential.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Hayden W. Craun
Academic Institution:	Virginia Tech
Major:	Computer Engineering
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Finish my undergraduate degree and possibly go to graduate school for electrical engineering
NIST Laboratory, Division, and Group:	PML, Microsystems and Nanotechnology, Photonics and Plasmonics
NIST Research Advisor:	Amit Agrawal
Title of Talk:	Design of Multiresonant Plasmonic Nanocavities for Label-Free Nonlinear Optical Voltage Sensing

Abstract:

Multiphoton voltage imaging with voltage-sensitive fluorophore molecules has been instrumental in monitoring deep-tissue electrophysiological activities but suffers from challenging issues, including photobleaching, phototoxicity, and disruption of native cellular behaviors. In this project, we investigate elliptical nanolaminate plasmonic nanoantennas (ENLPNAs) as label-free solid-state voltage nanosensors to produce polarization-dependent plasmon-enhanced second harmonic generation (PESHG) signals with high conversion efficiency and large voltage sensitivity. Utilizing finite-difference time-domain simulations, we take advantage of the resonant plasmonic properties of gold nanostructures to engineer multiresonant, elliptical nanocavities to produce PESHG signals. We achieve multiresonant response with optimized sub-wavelength metal-insulator-metal (MIM) building blocks. By manipulating key geometrical parameters of our nanostructure, we widely tune the nanostructure's resonances with multiple degrees of freedom. By combining these properties, we find conditions for cross-polarized spatial mode overlap to enhance PESHG signals. Based on these simulation results, we plan to fabricate ENLPNAs via electron-beam lithography and lift-off to measure their nonlinear optical response and voltage sensitivity. With the development of these label-free voltage nanosensors, we aim to broaden the interface between the biological system and integrated nanosystem to monitor network-level brain activities using standard multiphoton processes.

SURF Student Colloquium

NIST – Boulder, CO
August 2-4, 2022

Name: Aagam Dalal	
Academic Institution: University of Pennsylvania	**Major:** Computer Engeineering
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	(Career) Computing Hardware/Firmware
NIST Laboratory, Division, and Group:	PML, Applied Physics Division, Quantum Nanophotonics Group
NIST Research Advisor:	Dr. Krister Shalm
Title of Talk:	Testing and demonstrating a new toolkit for public randomness beacons

Abstract:

The NIST Randomness Beacon provides world-class public randomness based on the Interoperable Randomness Beacon project. The goal is to produce a source of randomness that sensitive applications such as voting protocols or lotteries can use. However, the current application programming interface (API) of the beacon needs improvement. In partnership with the University of Colorado at Boulder, a new randomness beacon is being launched to overcome this issue and is based on an easy-to-use Javascript interface called TwineJS.

In this talk, I will discuss my work testing and demonstrating the TwineJS library. The TwineJS library had not yet been thoroughly tested at the start of the summer. My first task was to write unit tests for TwineJS to test the API and remove bugs. During the second part of the project, I built a web game using the Vue javascript framework and TwineJS that demonstrates how to implement contracts based on a randomness beacon. In the real world, such contracts can help facilitate transparency and verifiability in allocating anything from admission into elite public schools to anti-corruption audits. In the web game, players try to predict the outcome of a coin flip, which is extracted from public randomness. As the game unfolds, users see the guarantees that Twine and the randomness beacon provide, and how they stop any player from having an unfair advantage. The results show how the NIST randomness beacon can be leveraged to build transparent applications.

SURF Student Colloquium

NIST – Boulder, CO
August 2-4, 2022

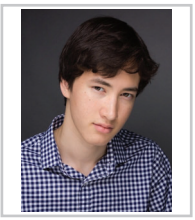
Name:	Will Dienstfrey
Academic Institution:	Amherst College
Major:	Physics
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Graduate school and pursue a career in atmospheric/geophysics
NIST Laboratory, Division, and Group:	Physical Measurement Lab, Applied Physics, Molecular and Bio-Photonics
NIST Research Advisor:	David Plusquellic
Title of Talk:	Monitoring Atmospheric Stability for Plume Emission Flux Measurements

Abstract:

Non-invasive, real time measurements of greenhouse gases (GHGs) at high-emission sources are critical for monitoring and regulation. It has been shown that one can observe emission flux of buoyancy-dominated smoke plumes using a Differential Absorption LIDAR system (DIAL). However, quantification of emission flux is challenging as variations in atmospheric conditions affect the shape, location, and density of the gas, which can lead to plume GHG concentration information becoming lost in the noise of ambient gas signal. Therefore it is important to point and adjust the DIAL beam to sample the optimal part of the plume. This work seeks to determine plume characteristics based on auxiliary atmospheric data to stabilize DIAL measurements of greenhouse gases.

We use a Gaussian dispersion plume model to model smoke plume characteristics as a function of atmospheric conditions. In turn, atmospheric variations are tracked in the model using Turner and Pasquill-Gifford stability classes which account for changes in factors such as wind speed and the net radiation index. Real world atmospheric data from a NOAA Doppler LIDAR system and a VAISALA point source instrument are used to test the model and understand the model uncertainties.

Atmospheric models face many challenges as there are numerous hidden interactions between parameters. We implement a Monte Carlo study to estimate uncertainty in smoke plume concentration predictions due to atmospheric variation. By introducing controlled stochastic variation in the input parameters, one can observe the statistical effect this variation has on the output. In our study, wind speed was varied, and the resulting concentration variations were determined via the model. This work found that the best time to observe a smoke plume is at night in stability classes 6 and 7. An interface using this model was constructed to help guide experimental measurements of the plume in real time.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name:	Michael Gabe
Academic Institution:	Case Western Reserve University
Major:	Physics
Academic Standing (Sept. 2022):	Physics BS (Graduated)
Future Plans (School/Career):	I plan on attending graduate school in either physics or astronomy Fall 2023, with the intention of pursuing some cosmological research.
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Quantum Optics Group
NIST Research Advisor:	Dr. Zachary Levine
Title of Talk:	Nonperturbative nonlinear optics in a rubidium vapor cell

Abstract:

Because of their ability to decrease shot noise, squeezed states of light have been a hot topic of research interest. They have famously been used to increase the sensitivity of LIGO's gravitational wave detector. Paul Lett has been examining relative-intensity squeezing by four-wave mixing in Rb-85 vapor. Lett's experiment in 2007 featured Ti:sapphire lasers sent through Rb-85 vapor, while his current experiment feeds laser components back through the Rb-85 vapor. The current experiment outputs an anomalous oscillatory effect in the amplitude of the laser. To further our understanding of this optical system, this project computationally models the experiments' induced dipole moment from Rb-85 D1 transitions due to excitations from the laser. As perturbation theory likely breaks down due to the laser's near-resonant tuning, our code calculates the density matrix in the time domain, which we will further analyze in frequency space using Fourier transformations. In this project, we verify the code by matching analytic solutions such as the Rabi frequency for an ideal two-level system, then calculate chi_zzzz and chi_xxzz for the Rb-85 vapor.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Michael Gutowski

Academic Institution: Villanova University | **Major:** Electrical Engineering

Academic Standing (Sept. 2022): Sophomore

Future Plans (School/Career): Pursuing Masters in Engineering

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Sensor Science Division, Dimensional Metrology Group

NIST Research Advisor: Braden Czapla

Title of Talk: Computer Vision Identification and Analysis of Interferometric Fringes

Abstract:

The Dimensional Metrology Group in the Physical Measurement Laboratory at NIST uses a specialized interferometer to precisely measure sphere diameters with nanometer uncertainty. This instrument, called the Strang Viewer, is crucial in the measurement of reference spheres used to calibrate equipment internally at NIST and for external customers, such as ball-bearing manufacturers.

The Strang Viewer's operating procedure includes capturing images of the fringe pattern created by the interference of laser beams reflecting between two optical flats, in between which the sphere is located. Encoded in the fringe pattern is the distance between the two flats. To access the information, the current analysis software requires the operator to identify key features in the images to assist the algorithm in its calculations. This method can be time-consuming and can possibly introduce human error into its calculations.

This project utilized computer vision techniques to automatically detect the positions of the sphere and fringes in the images, decreasing the potential for human error. The new algorithm also proved to be faster than the existing software. In the future, the new algorithm could be improved by implementing additional image filtering to enhance the identification of the fringes.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Samir Kulkarni	
Academic Institution: UC Riverside	**Major:** Physics
Academic Standing (Sept. 2022):	Sophomore
Future Plans (School/Career):	Graduate School
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Atomic Spectroscopy
NIST Research Advisor:	Dr. Joseph Tan
Title of Talk:	Simulating electron beam behavior in a miniature electron beam ion trap

Abstract:

Highly charged ions (HCIs), traditionally found in hot plasmas, may have colder applications, such as precise atomic clocks, probing fundamental physics, and quantum information processing. NIST has an electron beam ion trap (EBIT) with a magnetic field of approximately 3 T to facilitate the production of HCIs. An ongoing project at NIST is to create a more compact EBIT, or mini-EBIT, using NdFeB permanent magnets rather than large superconducting coils. This construction is more effective at creating HCIs with ionization energies lower than 1 keV. The highest charge states an EBIT can produce depends on the energy and current density of the electron beam. Using a program called LORENTZ, we will model the mini-EBIT, simulate the electron beam's space-charge-limited motion, and estimate the current density when passing high currents through the drift tubes of the mini-EBIT. The goal is to understand better the electron beam optics in the mini-EBIT and provide predictions to be compared to actual measurements for evaluating performance.

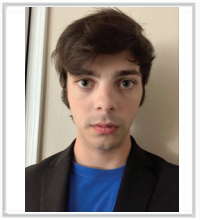
SURF Student Colloquium

NIST – Boulder, CO
August 2-4, 2022

Name:	Connor Lewis
Academic Institution:	Virginia Commonwealth University
Major:	Biomedical Engineering
Academic Standing (Sept. 2021):	Junior
Future Plans (School/Career):	VCU Guaranteed Admission Program for Medicine (BS/MD)
NIST Laboratory, Division, and Group:	NIST Boulder, Magnetic Imaging Group (MIG), Physical Measurement Laboratory (PML)
NIST Research Advisor:	Stephen Russek
Title of Talk:	Diffusion and Kurtosis in Brain Tissue Mimics

Abstract:

Diffusion based Magnetic Resonance Imaging (MRI) has increased due to its ability to non-invasively determine functional connectivity and tissue microstructure. Diffusion tensor imaging (DTI) relies on a Gaussian water diffusion model to determine general tissue structure including cell density and anisotropy. However, Gaussian diffusion models do not account for complex biological tissue structure and cell membranes that slow water transport. Kurtosis is a statistical technique to account for this non-Gaussian portion of water transport and is particularly present at high magnetic gradient strengths. The gradients are used to modulate spin densities on the micrometer scale and enable tracking of water motion at the cell level. Our goal was to model water diffusion in liposomal tissue mimics using a Monte Carlo water diffusion simulator. We measured the liposomal samples using nuclear magnetic resonance (NMR) pulse sequences to obtain T1 and T2 spin relaxation times, and water diffusion signatures. The diffusion signature consists of a normalized integrated signal versus gradient strength as parameterized by the b-value. An oscilloscope measured the gradient strength throughout data collection and provided an accurate calculation of the b-value for each pulse sequence. Disimpy, a Monte Carlo GPU based simulator was used to calculate diffusion signatures of liposomal mesh structures, where liposomal size varied from 100 nm to 1000 nm. Water molecules were randomly placed, and simulations using identical pulse sequences used on the NMR were performed in order to track water movement and signal evolution. The simulations output normalized integrated signal versus b-value showed kurtosis similar to the liposomal samples. Different liposomal structures were compared with the NMR data to understand how the diffusion signatures were related to the underlying microstructure. Modeling and simulations of the liposomal mesh is ongoing to correlate NMR/MRI diffusion data with underlying tissue microstructure. Better analysis of diffusion signatures can be used to determine overall tissue health, tumor type, tumor cell aggressiveness, and response of tumors to therapy.



SURF Student Colloquium

NIST – Boulder, CO

August 2-4, 2022

Name: Gabriel Lewis	
Academic Institution: University of Kansas	**Major:** Physics
Academic Standing (Sept. 2021):	Senior
Future Plans (School/Career):	Looking to Earn a Master's in Nuclear Physics Interested in Researching/Procuring Experimental Nuclear Fuel Rods
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Electromagnetics, Spin Electronics Group
NIST Research Advisor:	Matthew Pufall
Title of Talk:	Normal Modes of Nanoscopic Ferromagnets

Abstract:

The normal modes of ferromagnets can be coupled to electromagnetic waveguides to make electronic circuit elements like microwave filters, circulators, oscillators, and as part of transducing microwave-to-optical signals using strong coupling between a ferromagnet and a resonator. The resonances or "normal modes" of ferromagnetic structures are difficult to calculate. Ferromagnets made of iron, nickel, cobalt, and rare earth metal have a large magnetic moment even without the presence of an externally applied magnetic field, which produces a self-field that complicates calculation of the resonance frequencies of patterned magnetic elements. Recent measurements have shown a series of modes that were not expected from analytical methods, necessitating computation using numerical methods.

We use MuMax3 micromagnetic code to numerically simulate magnetization dynamics of a range of small (sub-micrometer) ferromagnetic, prisms. MuMax3 uses the speed and parallelism of graphics processing units to speed up simulation time over those ran on CPUs. A script sets up the magnetic environment consisting of a magnetic structure, and both constant and time-varying applied magnetic fields. MuMax3 uses finite-element methods, so the ferromagnetic object is discretized into smaller (nanometer-scale) elements to capture nanoscale dynamics. The magnetization as a function of time and space is then determined by numerically integrating the Landau-Lifshitz-Gilbert equation. This determines the magnetization of the system, and how it changes over the course of the simulation. From the data calculated from MuMax3, we can apply a Fast Fourier Transform to see normal modes, which appear as peaks in the gigahertz range of frequency space.

We find that the simulations conducted reasonably correlate to the frequencies of the fundamental mods and spacing of the higher order modes. In my talk, I will describe how these normal modes depend on the shape and composition of the ferromagnetic element.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Faith Makumbi

Academic Institution:	University of Kentucky	**Major:**	Physics
Academic Standing (Sept. 2022):	Senior		
Future Plans (School/Career):	Go to graduate school		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science, Remote Sensing		
NIST Research Advisor:	Susana Deustua		
Title of Talk:	Examining the Thermal Properties of an Artificial Star for Flux Calibration		

Abstract: An important aspect of modern observational cosmology is that data must be precise and accurate. For example, to measure the properties of dark energy using Type Ia Supernovae with an uncertainty of 1% or less means that the calibration of supernova color must be no greater than 0.5%. Astronomers use color to represent the ratio of light measured through any two band passes (filters). Currently, the uncertainty in color is limited by how well the stars used as standard candles are calibrated. One way to improve flux calibration techniques of modern telescopes entails utilizing an artificial star whose light output is well characterized and traceable to the SI standards. The artificial star can then be used to calibrate real stars. Stars are suitable calibration standards because of their numerosity and easy availability. The focus of my research is to study the design of a prototype artificial star known as CANDLE (Calibration using an Artificial star with NIST-traceable Distribution of Luminous Energy). CANDLE is a proposed instrument that will be designed to go on a small satellite in space, and project light calibrated to a telescope. I am using COMSOL to simulate the thermal properties of CANDLE under different configurations. This study will provide a better understanding of CANDLE' s thermal properties under different conditions and be used to inform the final design of the payload.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Evan McClintock			
Academic Institution:	University of Maryland College Park	**Major:**	Physics, Computer Science
Academic Standing (Sept. 2022):	Junior		
Future Plans (School/Career):	Graduate School, Physics and CS research		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory		
NIST Research Advisor:	Dr. Richard Steiner		

Title of Talk: Automating instrumentation for the calibration of DC power meters

Abstract:

In recent years, DC power usage has become increasingly common, driven by renewable energy sources and electric vehicle charging. However, the need for precise DC power meter calibration is not yet met. In this project, we begin fabricating a method to meet this demand. To ensure resulting uncertainty on the order of tens of ppm, all elements of the final setup must individually maintain high degrees of precision. Reliable methods of automatically recording and analyzing large amounts of data are vital in reducing the uncertainty in these calculations and are therefore a large focus. We have concentrated primarily on the calibration of a DC voltage source and current transducer. The source must have correction coefficients developed and usable up to 1V, building off previous SURF work with the Fluke 8588A multimeter. The corrections for the transducer must be known up to 100A. It requires a voltage source to set the output of a current transconductance amplifier and measurement of the corresponding voltage from the current transducer and across a low-ohm shunt resistor, the latter of which is dependent on temperature from self-heating. The results of this project will serve as a foundation for following work, allowing completion of the calibration of DC power meters with high degrees of precision.

Disclaimer: Any mention of commercial products within this paper is for information only; it does not imply recommendation or endorsement by NIST.

SURF Student Colloquium

NIST – Gaithersburg, MD

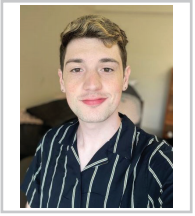
August 2-4, 2022

Name: Shawn Meyer		
Academic Institution: University of Texas at Austin	**Major:** Physics	
Academic Standing (Sept. 2022):	Senior	
Future Plans (School/Career):	Graduate School or Industry Research	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Nanoscale Device Characterization Division, Atomic Scale Device Group	
NIST Research Advisor:	Richard Silver	
Title of Talk:	Analysis of Dopant Quantum Dots in Silicon	

Abstract:

Strong electronic interactions in quantum materials are responsible for phenomena such as high-Tc superconductivity or Mott insulators The Fermi-Hubbard model provides a low-energy description of electrons and is believed to have the ingredients to explain such exotic behaviors. The model consists of a lattice of sites where electrons are situated, allowed hopping between nearest-neighbor sites, and an interaction term representing the Coulomb repulsion between, which can be long-range. However, solutions of the model in its generic form are not accessible to current theory or numerics. It has been shown that arrays of dopant quantum dots in Silicon effectively simulate the Hubbard model. With the ability to place atoms with atomic precision using scanning tunneling microscopy, it is possible to make arbitrary lattices and tune hopping and interaction parameters for electrons.

We analyze a two-by-two array of quantum dots with four gates to vary the chemical potential landscape, and source and drain leads to allow electrons to tunnel onto or off the array. The primary focus is to establish a connection between device parameters and those of the Hubbard model by comparing a simulation of the quantum dot device to experimental data. However, we also explore the effects of disorder in the system; this is important because fabrication can be imprecise. We use the open-source Python package QmeQ to construct the Hamiltonian of the system and by finding its ground states, map out the electronic configurations as the gate voltages are varied. QmeQ gives us a test bed to tune parameters such that the experiment and simulation agree.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Daniel Quinter	
Academic Institution: Brown University	**Major:** Physics
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Currently intend to attend graduate school for a PhD in a physics program.
NIST Laboratory, Division, and Group:	PML, Quantum Measurement Division, Laser Cooling and Trapping Group
NIST Research Advisor:	Dr. Charles Clark
Title of Talk:	Quantum Random Number Generation in Trapped-Ion Computing with Error Mitigation

Abstract:

In the field of cryptography, random number generators provide a consistent method for generating secure keys which serve as the backbone of encryption. Quantum random number generators (QRNGs) offer an appealing path toward true randomness and consequently greater cryptographic security, motivated by relatively simple quantum mechanical principles. Unfortunately, computations including the generation of secure keys or bitstrings via projective measurement are hampered by noise present in real-world quantum circuits. The predictability and consistency of this noise across experiments reduces the overall entropy of any key generated in this fashion. We thus investigate the statistical randomness of bitstrings encoded by quantum cryptography protocols utilizing the cloud-based trapped-ion computers of IonQ in College Park, Maryland.

In this talk, I will discuss noise mitigation techniques and performance results for quantum random number generation using a variety of circuits on IonQ's backend. Mitigation is achieved through several techniques, chiefly calibration and general error mitigation, with each technique demonstrating some level of error mitigation which is quantified and compared. In order to assess the efficacy of each form of mitigation, they are applied to random quantum circuits of varying depths, with special emphasis placed on GHZ and W-state circuits due to their attractive entanglement properties. Preliminary findings demonstrate positive noise minimization, but on a low order of magnitude, partly due to the relatively high fidelity of quantum states generated by the IonQ backend. These approaches are then applied to the randomly generated bitstrings in order to determine whether or not error mitigation can cause an increase in statistical significance for the results of any given randomness test.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Satvik Manjigani

Academic Institution: University of Maryland, College Park | **Major:** Physics and Astronomy

Academic Standing (Sept. 2022): Junior

Future Plans (School/Career): I plan to pursue a degree in graduate school, followed by research in either academia or the private sector.

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Microsystems and Nanotechnology Divison, Biophysical and Biomedical Measurement Group

NIST Research Advisor: Michael Zwolak

Title of Talk: Characterizing DNA Structures with Machine Learning

Abstract:

Modern advances in machine learning allow for the rapid automation of classification (unsupervised) and prediction (supervised) procedures, which has the potential to expedite biophysical and biomolecular research considerably. The classification of biomolecules based on distinct physical parameters has a particular application in studying proteins for drug development. Here, we use a Convolutional Neural Network to predict physical binary states (i.e. folded vs. unfolded, high vs. low temperature) of simulated DNA sequences using time series data. Specifically, we calculate the radius of gyration of the DNA for 1 μs of real time, and adjust the neural network to improve the machine learners' performance. This work serves as a baseline that can be expanded to characterize biomolecules into more classes using different physical properties.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Abrar Sheikh	
Academic Institution: Yale University	**Major:** Chemical (ABET) & Electrical Eng.
Academic Standing (Sept. 2022):	GPA 3.97
Future Plans (School/Career):	Masters/Ph. D
NIST Laboratory, Division, and Group:	Thermodynamic Metrology Group, NIST
NIST Research Advisor:	Dr. Stephen Eckel
Title of Talk:	Progress Towards Validation of the Cold-Atom Vacuum Standard

Abstract:

We took a series of measurement to validate operation of the portable cold-atom vacuum standard (pCAVS). The pCAVS measures vacuum in the ultra-high vacuum (UHV, <10e-6 Pa) and extreme high vacuum (XHV, <10e-9 Pa) ranges by observing the loss rate of cold atoms trapped in a shallow magnetic quadrupole trap due to collisions with the background gas. In these regimes, the pressure p is related to the decay rate Γ by the equation p = ΓkT/K, where T is the temperature of the background gas, k is the Boltzmann constant, and K is the rate coefficient, which is species dependent. This equation is true assuming that there are no other sources of loss than collisions with background gas molecules. Other types of loss include evaporative loss, where collisions between the cold lithium atoms results in some being ejected from the trap, and Majorana (spin-flip) loss, which occurs when the atom approaches the center of the trap (and the magnetic field suddenly reverses direction) so that the atom's magnetic dipole is now misaligned with the magnetic gradient of the trap. We measured decay rates at known pressures to experimentally determine K for argon, nitrogen, and helium, and compared these values to theory. Moreover, we searched for systematic effects due to imaging, Majorana loss, evaporative loss, and other effects. It appears that Majorana loss at the trap center is minimal. Evaporative losses are estimated to contribute a few percent error to any pressure measurement from the pCAVS. We present our preliminary results on experimental determinations of K, and compare them with theory.

SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Hunter Staiger	
Academic Institution: Clemson University	**Major:** Electrical Engineering
Academic Standing (Sept. 2022):	Senior
Future Plans (School/Career):	Attending graduate school in order to become a professor.
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Atomic Spectroscopy Group
NIST Research Advisor:	Yuri Ralchenko
Title of Talk:	An automatic calibration algorithm and the efficiency determination of the NIST spectrometer.

Abstract:

Extreme ultraviolet (EUV) radiation is produced by transitions between energy levels of highly charged ions. By precisely measuring the wavelength of the emitted radiation, valuable information about the atomic structure can be obtained and compared to the most advanced quantum theories. Theories today are so precise that uncertainty in the size of the atomic nucleus is the primary limiting factor in the calculations. Therefore, precisely comparing EUV experiments and theory can determine nuclear parameters.

At NIST, EUV wavelengths are measured using a spectrometer, but factors such as temperature variation and the spectrometer's position can significantly impact the daily calibration. Additionally, the detection efficiency of the spectrometer varies with the wavelength of incoming radiation. The changing efficiency can affect the measured line intensities and even systematically shift the measured wavelength. In the past, time-intensive calibrations were completed manually, and the efficiency curve was approximated using ray-tracing software. To improve the precision of EUV wavelength measurements, a novel automatic calibration algorithm was developed and implemented over a database of NIST data. The efficiency curve of the spectrometer was reconstructed by comparing theoretical and experimental relative intensities.

Overall, the automatic calibration method produces precision comparable to or better than manual calibrations in a fraction of the time. Utilizing the efficiency curve in the calibration process seems to produce minimal systematic shifts. The generality of the automatic calibration algorithm suggests that similar methods can be implemented with other instruments in the spectroscopy field, reducing the time needed to analyze complex data. Shortly, I aim to distribute the automatic calibration software in an easy-to-use format to assist the experimental work done by NIST's atomic spectroscopy group.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-4, 2022

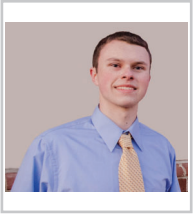
Name: Grace Tang		
Academic Institution:	Cornell University	**Major:** Electrical and Computer Engineering
Academic Standing (Sept. 2022):	Sophomore	
Future Plans (School/Career):	Complete undergraduate degree, possibly graduate school	
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Nanoscale Device Characterization Division, Nanoscale Processes and Measurements Group	
NIST Research Advisor:	Katelyn Goetz	
Title of Talk:	Evaluating Organic Thin-Film Transistors and Processing Methods	

Abstract:

Organic field-effect transistors (FETs) are devices in which the semiconductor layer consists of an organic material such as a polymer or small molecule. Unlike silicon-based transistors, they be processed at room temperature from solution and can therefore be manufactured on flexible surfaces such as plastics and textiles. This allows for a variety of applications, such as bendable high-resolution color displays, wearable electronics, non-invasive health-monitoring systems, and more.

The goal of this project is to reduce the amount of time it takes to process device data, leading toward high-throughput experimentation. To do so, we wrote MATLAB code to process data for many devices at once, accurately extracting four figures of merit - the charge-carrier mobility, threshold voltage, subthreshold slope, on/off current ratio – without the need to observe every curve. Because the mobility in particular is prone to inaccurate estimation if the devices are non-ideal, we fit this parameter by first determining the interval on which to fit it using the second derivative. Then a linear regression was found on this interval, whose slope was used to calculate mobility. In addition, we calculated a reliability factor to describe how far the fitted value deviates from the ideal. The resulting data was then displayed in a heatmap that allows us to compare these parameters for different transistor channel lengths.

With remaining time, we are developing strategies to programmatically correlate features of the semiconductor microstructure, such as grain size and alignment, with the electrical parameters. Some potential ones include finding the angle streak patterns make with the FET channel and the line intercept method, through which counts the number of grain boundaries that intersect a line. By doing so, we want to find the processing parameters that would allow for the largest margin of error. This would make manufacturing easier since it can be less precise. By making it easier to manufacture high quality organic transistors, not only would we make their performance comparable to or better than silicon-based FETs, but we would also expand the applications where they can be used.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

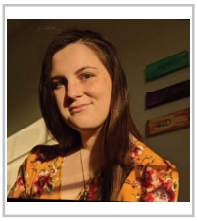
Name: Travis White Jr.

Academic Institution: Mercer University | **Major:** Mechanical Engineering

Academic Standing (Sept. 2022):	Sophomore
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, Metric Program
NIST Research Advisor:	Elizabeth Benham
Title of Talk:	Metric Program Resource Development

Abstract:

Utilizing the International System of Units (SI) in the United States provides an opportunity to significantly increase efficiency and decrease unit errors in trade and commerce. The Office of Weights and Measures Metric Program aims to develop and publish informational and educational resources for U.S. students, teachers, businesses, government, and the public. Throughout the SURF Program, a centralized curation of metrication websites has been developed to inform the Metric Program's audience of potential benefits and risks related to metric system conversion. A webpage template was developed and implemented for NIST's educational STEM registry, NEST-R, to permit detailed article entries on the public website. With this template, multiple entries have been created for existing SI education publications. Additionally, metrication inquiries from U.S. businesses, Congress, and international government representatives have been analyzed to ensure that the new websites included appropriate information for these technical requests. These resources developed for the Metric Program provide solutions that will be instrumental in education outreach and stakeholder engagement for learning and implementing the International System of Units.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Lucy Yagodich

Academic Institution: Penn State University-Harrisburg | **Major:** Electrical Engineering

Academic Standing (Sept. 2022): Senior Undergraduate Student

Future Plans (School/Career): I plan to have a career in medical imaging and/or nuclear medicine.

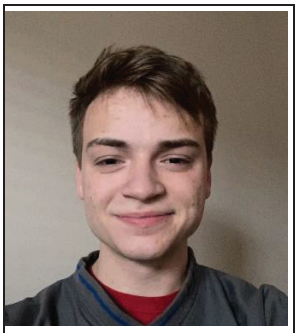
NIST Laboratory, Division, and Group: Physical Measurement Laboratory- Quantum Measurement Division

NIST Research Advisor: Dr. Angela Hight Walker

Title of Talk: Interconnecting and Controlling In-Operando Spectroscopic Measurements

Abstract:

Quantum materials characterized with Raman spectroscopy involves the excitation of samples with a specific laser wavelength (or color) and collection of inelastically scattered light (Raman process), uniquely at NIST, as a function of polarization, temperature, magnetism, and applied electric fields. Yet any contiguous operation of instrumentation that controls experimental conditions such as temperature and magnetism often involve use of several distinct proprietary programs and devices. Here, I present my work in the design and development of a highly customized LabVIEW program (named MagnetoRaman Spectroscopic and Electrical Measurement System "MrESMS") that consolidates the control and operation of three independent instruments: Raman spectrometer (HORIBA JYT64000), a cryostat with a superconducting magnet (attocube attoDRY 2100), and a source measurement unit (Keithley 2400). Using the MrESMS program, we demonstrated successful remote control and automated measurements with the cryostat and source measurement unit (SMU). A device made from an exotic 2D quantum material 2M-WS2 was measured for the demonstration. We showed that the program is capable of measuring the superconducting transition as well as the dependence of the transition temperature as a function of applied magnetic field. The MrESMS is designed for expandability such that the addition of the Horiba spectrometer, or any other additional future devices, will be relatively seamless.



SURF Student Colloquium

NIST – Gaithersburg, MD

August 2-4, 2022

Name: Joshua Young		
Academic Institution:	University of Kentucky	**Major:** Physics
Academic Standing (Sept. 2022):	4.0	
Future Plans (School/Career):	Graduate School, Teaching/Private Sector	
NIST Laboratory, Division, and Group:	PML, Radiation Physics Division 682, Dosimetry Group	
NIST Research Advisor:	Dr. Ronald Tosh	
Title of Talk:	Development of an Open-Source Workflow for End-to-End Simulation of an Ultrasonic Calorimeter for Imaging of Radiation Dose.	

Abstract:

Radiotherapy for cancer treatment seeks to deliver radiation dose to tumors while sparing surrounding healthy tissue. Such spatially variable dose fields differ significantly from the highly uniform fields used to calibrate detectors, which introduces large systematic uncertainties in measurements of dose delivered to patients and concomitant risks for safety and effectiveness of therapeutic radiation. To address this, NIST is working on a primary standard for dose calibration that works in nonuniform fields. One embodiment involves the use of ultrasonic imaging of temperature distributions in water. An experimental prototype developed here has demonstrated proof of principle, but speedups in data acquisition and image processing are necessary to make it practicable for eventual use as a new standard. The present project is developing computational tools to aid the design process, consisting of finite-element analysis to simulate dose delivery to a water phantom, discrete sampling of that dose distribution to simulate data acquisition, and image reconstruction based on the simulated acquired data. It is expected that this work will provide needed tools for optimizing sensor arrays and image processing algorithms to affect the needed speedups.

SURF Student Colloquium

NIST – Boulder, CO
August 2-4, 2022

Name:	Helen Zhang
Academic Institution:	University of California, Berkeley
Major:	Biology, Data Science
Academic Standing (Sept. 2022):	Junior
Future Plans (School/Career):	Graduate school
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Applied Physics Division, Molecular and BioPhotonics Group
NIST Research Advisor:	Jeeseong Hwang
Title of Talk:	Hyperspectral Imaging for Tumor Margin Analysis in Breast Tissue Resection

Abstract:

Breast lumpectomy is a surgical procedure that removes cancerous tissue with a margin of healthy tissue around it to ensure that all tumorous tissue is removed. 32-63% of breast cancer patients are recalled to a second surgery due to incomplete removal of the tumor, which is costly and reduces the quality of life of patients. To analyze tumor margins, pathology imaging and dark-field hyperspectral microscopy were applied. Pathology imaging was used to categorize tissue and confirm a tumor margin. Dark-field hyperspectral microscopy was implemented to image the tumor margin in resected human breast lumpectomies. Normal and cancerous tissue cases were collected using the hyperspectral imaging technique, which produces a hyperspectral data cube made up of a reflectance spectrum and a series of narrow and contiguous wavelength bands. The spectral angle mapper classification technique was employed to quantify the similarity between a reference image and an unknown image. The alpha value formulated in the spectral angle mapper is the spectral correlation angle formed between the reference spectrum and the image spectrum. For each tissue type, the optimal alpha value was determined through an alpha validation process. Based on histological annotation, regions of interest were taken to extract endmembers, the set of spectrally unique surface materials existing within an image. The alpha value was adjusted with samples of non-cancerous tissue and then validated by generating a spectral angle mapper classification image on the original cancerous tissue image to ensure a match to the pathology interpretation. Adjustment of the alpha value was found to control tumor margin detection. Extended alpha value validation against a broader range of tissue types enhanced tumor margin detection by minimizing data errors and improving the accuracy of tissue classification. Thus, the alpha value can serve as a biomarker and measurable indicator of biological conditions.