SURF

Summer Undergraduate Research Fellowship

Colloquium 2021

Greetings,

On behalf of the Director's Office, it is my pleasure to welcome you to the 2021 SURF Colloquium. Unlike previous colloquiums, this program is occurring 100% virtually.

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, #2021SURFProgram.

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 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	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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Summer Undergraduate Research Fellowship (SURF) Colloquium Plenary Session

Tuesday, August 3, 2021 (10:00 AM to 11:40 PM (ET))
Meeting Link: https://primetime.bluejeans.com/a2m/live-event/abyktxzj

Time (ET)	Session Information
10:00 AM	**Welcome**
	Session Moderator: Brandi Toliver
10: 15 AM	**Communication Technology Laboratory (CTL)** *Sreyas Sabu Chacko* A study of the properties belonging to the Articulation Band Correlation Modified Rhyme Test
10:30 AM	**Engineering Laboratory (EL)** *Cameron Busser and Riya Sharma* Emergency Communication During Hurricane Maria
10:45 AM	**Information Technology Laboratory (ITL)** *Jason Eveleth* Grain coarsening in Voronoi diagrams
11:00 AM	Break
11:10 AM	**Material Measurement Laboratory (MML)** *Jordan Hoffman* Determination of Strain Path Envelope in an Optimized Cruciform Specimen of AISI 1008 Steel
11:25 AM	**NIST Center for Neutron Research (NCNR)** *Claire Lamberti* Broad-Spectrum Antibiotic Glasses with Tunable Solubility
11:40 AM	**Physical Measurement Laboratory (PML)** *Katherine Slattery* Conditions for a Single Photon Echo

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Tuesday, August 3, 2021 (1:00 to 2:30 PM (ET))

	Communication Technology Lab (CTL)	**Engineering Laboratory (EL)**	**Information Technology Laboratory (ITL)**
	Moderator: TBD	**Moderator: TBD**	**Moderator: Derek Juba**
Time	Meeting Link: https://bluejeans.com/807706899/0663	Meeting Link: https://bluejeans.com/455089596/4825	Meeting Link: https://bluejeans.com/649812750/4953
1:00 PM	*Megan Lizambri* NetSimulyzer - A 3D Network Simulation Analyzer for ns-3	*Donald Chang* A Review of Heat Flux Measurements in Large Wildland Experiments	*Robert Bennett* Analysis of Biomedical Image Segmentations - Low-Field MRI
1:15 PM	*Marckie Zender* Mission Critical Voice Quality of Experience GUI	*Noelle Crump* Modeling Windflow Over Large-scale Complex Geometries	*Elvin Liu* Evaluation of the FogBank cell segmentation method ported to Python
1:30 PM	*Viktor Murray* Automated Unit Testing of Voice Quality of Experience Tools	*Derek Schoenberger* A Case Study of Modeling Machine Tool Systems using Standards	*Raymond Karyshyn* Comparative Evaluation of XML and JSONL for Technical Data
1:45 PM	*Robert Xu* Eliminate the Man-in-the-Middle: 5G Edge Security	*A'di Dust* Generalized Procedural Generation With Measured Alteration For Robot Agility	*Muktaka Joshipura* Streaming Linear Algebra
2:00 PM	*Carolina Whitaker* Image Quality for Computer Vision	*Jonathon Gruener* Development of tracking software for fiber-reinforced polymer composite and concrete samples	*Nizar Benmohamed* High-Performance Python
2:15 PM		*Prasun Guragain* Web-based software for investigating and evaluating data tampering	*John Kucera* Investigation of Floating-Point Reproducibility
2:30 PM	Break		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Tuesday, August 3, 2021 (2:40 to 4:10 PM (ET))

	Engineering Laboratory (EL)	**Information Technology Laboratory (ITL)**	**Material Measurement Laboratory (MML)**
	Moderator: TBD	**Moderator: Lotfi Benmohamed**	**Moderator: Ashley Green**
Time	Meeting Link: https://bluejeans.com/455089596/4825	Meeting Link: https://bluejeans.com/649812750/4953	Meeting Link: https://bluejeans.com/471510305/3535
2:40 PM	*Andrew Hoffpauir* A Biofidelic Impact Dummy to Evaluate the Safety of Collaborative Robot Applications	*Nina Agrawal* Identifying Carbon Nanotubes Using Machine Learning	*Jennifer Li* Evaluation of Carbon Nanomaterial Bioaccumulation Studies and Methods
2:55 PM	*Keely Hutchinson* Improvements in Laser-Powder-Bed-Fusion Additive Manufacturing Using Open-Platform Software	*Erchis Patwardhan* Implementing Parameterised Map Construction for use in Backpropogation Algorithm	*Katherine Dura* Assessing Structural Effects of RNA Modifications in Molecular Dynamics Simulations
3:10 PM	*Eugene Jeong* Comparison of Segmentation Methods for an Additively Manufactured Surface	*Denis Liu* cuML Benchmark Evaluation on Nisaba GPU Platform	*Michaela Staab* Data Analysis Methods to Describe Molecular Conformational Ensembles
3:25 PM	*Yekta Kamali* Performance analysis of a position verification sensor for robot workcell health degradation assessment	*Nishaant Goswamy* Named Data Networking (NDN) Dissector for Wireshark	*Catherine Gill* Understanding the Importance of the Peptide Chain in Representatively Modeling teClpS Binding Preference
3:40 PM	*Swathi Kashi* Energy-based Seismic Assessment Criteria	*Lindsay Susan Jones Marean* Inter-Annotator Agreement for Recognizing Ultra Fine-grained Entities	*Malaak Saadah* High-throughput Machine Learning for Chemical Informatics
3:55 PM	*Sahil Kochar* Web-based Tool for Service Life Prediction of Photovoltaics and Building Materials	*Joshua Zarb* Indicating relevance in search engine evaluation	*Katherine Boyd* Estimating HDX-MS of ERK2 from multi-microsecond molecular dynamics simulations
4:10 PM	Break		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Tuesday, August 3, 2021 (4:20 to 6:05 PM (ET))

	Engineering Laboratory (EL)	**Information Technology Laboratory (ITL)**	**Material Measurement Laboratory (MML)**
	Moderator: TBD	**Moderator: Annie Sokol**	**Moderator: Lilian Johnson**
Time	Meeting Link: https://bluejeans.com/455089596/4825	Meeting Link: https://bluejeans.com/649812750/4953	Meeting Link: https://bluejeans.com/471510305/3535
4:20 PM	*Alexander Kuan* Data Curation Tool Development and In-Situ Monitoring Data Analysis for Additive Manufacturing	*Peter Shin* Evaluating Augmented/Virtual Reality Visual Performance	*Miyu Mudalamane* Demonstrating SciServer Applications for Additive Manufacturing Benchmark Data
4:35 PM	*Aeron Liss* Photovoltaic Cell Processing and Calibration Using Electroluminescence Hyperspectral Imaging Measurements	*Karol Sadek* Designing Experiments to Estimate the Non-linear Response of a Spectroradiometer	*Noah Hobson* Applying Natural Language Processing to the NIST Public Data Repository
4:50 PM	*Reza Manuel Mirzaiee* Retargetable Animations for Industrial Agumented Reality	*Selena Xiao* Using Natural Language Processing to Supplement a Cyber Incident Graph Database	*Priya Shah* Research and Development of the NexusLIMS
5:05 PM	*Erik Mitchell* Prediction of Energy Consumption in Residential Homes using a Reinforcement Learning Algorithm	*Justin Chen* Client Development for the Entropy Source Validation Server	*Maurice Curran* Natural Language Processing for Standardizing Vocabulary in an Electron Microscopy Schema
5:20 PM	*Isaac Park* Beta Testing Unstructured Geometry within FDS using Pyrosim	*Khar Casse* Analyzing the Engagement of the K-12 Community in Cybersecurity: Past Efforts and Future Directions.	*Devin Golla* Modeling the Structure-Property Relationships of Diblock Copolymer Architectures
5:35 PM	*Patrick James* Analysis of Key Wall Characteristics in FRP Retrofitted Shear Wall Database	*Matteo Marchi* Web Archiving NIST's iNet with Brozzler	*Ethan Chen* Modeling Polycarbonate Confined Between Crystalline Silica Surfaces
5:50 PM	*Amaan Rahman* Markerless Human Kinematic and Kinetic Evaluation with 3D Monocular Pose Estimation Algorithms		*Eleanor Grosvenor* Computational Modeling of Commercial CO2 Electrolyzers Equipped with Nanostructured Cathodes
6:05 PM	End of Day		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Wednesday, August 4, 2021 (10:00 to 12:00 PM (ET))

	Engineering Laboratory (EL)	**Information Technology Laboratory (ITL)**	**Material Measurement Laboratory (MML)**
	Moderator: TBD	**Moderator: Tim Burns**	**Moderator: Carelyn Campbell**
Time	Meeting Link: https://bluejeans.com/455089596/4825	Meeting Link: https://bluejeans.com/649812750/4953	Meeting Link: https://bluejeans.com/471510305/3535
10:00 AM	*Nathan Rand* Data Specification for AM Machine Performance Tests	*Sophia Koh* Improving Machine Learning Heuristic Metrics for Solitonic Excitation Classification for Bose-Einstein Condensates	*Jalen Garner* Effect of Mechanical Strain on the Electronic and Magnetic Properties of UTe2
10:15 AM	*Dominique Regli* Cutting Force Monitoring for Smart Machine Tools	*Peter Lef* Denoising and Inpainting Material Microstructure Orientation Maps using Differential Equations	*Jesse Ji* Modeling Creep in Co-based Superalloys with AI
10:30 AM	*Lucia Rhode* Annotated Dataset for Exoskeleton Pose Estimation and Fit Evaluation	*Isabel Agnostino* Star Discrepancy	*Wyatt Gibbs* Procedural Polymer Morphology Generation for Resonant Soft X-Ray Scattering Simulations (RSoXS)
10:45 AM	*Thomas William Roche* Buyout Programs for Community Resilience	*Elizabeth Euwart* Probability Distribution of Number of Steps in Walk on Spheres Method	*Logan Saar* Bayesian Analysis based Active Learning System for Autonomous Physical Science
11:00 AM	*Mary Ruxsarash* Statistical Analysis of Condition Monitoring Test Data from Accelerated Aged Nuclear Power Plant Electrical Cables	*Ramon Suris-Rodriguez* Integral and q-Integral Representations of Askey-Wilson Polynomials	*Alex Wang* Benchmarking Active Learning Strategies for Materials Optimization and Discovery
11:15 AM	*Michael Shao* Better Hurricane Preparedness and Recovery through Data Analysis and Predictive Algorithms	*John Bodenschatz* Relations Between Carlson's Symmetric Elliptic Integrals and Legendre's Incomplete Elliptic Integrals	*Richard Ma* Use of Bayesian Inference to Plot Parameter Probability Distributions for High-Entropy Alloys
11:30 AM	*Emily Shimabukuro* Visualization of Traceability Data	*Timothy Mooney* Lefshetz Thimble Quantum Monte Carlo for Spin Systems	
11:45 AM	*Mackenzie Smith* Using X-ray Diffraction to Predict Cement Expansion from Sulfate Attack	*Marc Burlina* Image Fusion Methods for Fluorescence Guided Surgery	
12:00 PM	Break		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Wednesday, August 4, 2021 (1:00 to 2:30 PM (ET))

	Engineering Laboratory (EL)	**Material Measurement Laboratory (MML)**	**Physical Measurement Lab**
	Moderator: TBD	**Moderator: TBD**	**Moderator: Robert McMichael**
Time	Meeting Link: https://bluejeans.com/455089596/4825	Meeting Link: https://bluejeans.com/471510305/3535	Meeting Link: https://bluejeans.com/403818615/5811
1:00 PM	*Bethany Taylor* Semi-automated Building Commissioning using HVAC-Cx	*Bliss Han* Understanding Self-assembly of Programmable Polycrystalline Films	*John Lundstrom* Non-Linear Optimization for Enhanced Parameter Retrieval in Magnetic Resonance Fingerprinting
1:15 PM	*Ashley Tisaranni* Artificial Intelligence for Manufacturing Robotics	*Daniel Markiewitz* Designing colloidal crystals from functionalized polymer frameworks.	*Max Hanrahan* Calibration of Three-Axis Accelerometer and Gyroscope Using Pendulum-Based Excitation
1:30 PM	*Tyree Warren* Peg in Hole Assembly	*Alexandria Brady-Mine* Uncertainty Quantification in Transition-Matrix Monte Carlo Simulations	*Joe Cavanagh* The Ultimate Coin Flipper
1:45 PM	*Matthew Weiss* Multi-Robot Control Through CRPI Interface	*Ilyas Adnane* Calculating Entropies and Identifying Key Elements of Liquid Structure with Normalizing Flows	*James Vouzikas Jr* Automation of a hyperspectral confocal laser scanning microscope
2:00 PM	*Brian Woo-Shem* Occupancy-Based Heating & Cooling Control to Increase Residential Energy Efficiency	*Anika Rajamani* Developing R&R Tools for AI	*Jayden Craft* Sequential Bayesian Experiment Design
2:15 PM	*Divya Hadavale* Impacts of Complex Events		*Sadie Chafin* Automation of a hyperspectral confocal laser scanning microscope
2:30 PM	Break		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Wednesday, August 4, 2021 (2:40 to 4:10 PM (ET))

	Engineering Laboratory (EL)	Material Measurement Laboratory (MML)	Physical Measurement Lab (PML)
	Moderator: TBD	**Moderator: TBD**	**Moderator: Yaw Obeng**
Time	Meeting Link: https://bluejeans.com/455089596/4825	Meeting Link: https://bluejeans.com/471510305/3535	Meeting Link: https://bluejeans.com/403818615/5811
2:40 PM	*Alex Dai* Continuous Integration for Collaborative Web Documentation: Updating the AI-COI Catalog	*Sareet Nayak* Modeling Flow Birefringence of fd-Virus Solutions through a Microfluidic Channel	*Kendall Zammit* Mining of Solder Joint Reliability Data to Identify Possible Precursors to Catastrophic Failure
2:55 PM	*Samay Govani* Interfaces for Human-Robot Interaction	*Chloe Taylor* Large Interlayer Exchange Coupling in Ir-based Synthetic Antiferromagnets	*Richard Jinschek* Characterization of Fluke 8588 Reference Multimeter to Digitize and Analyze Power Data
3:10 PM	*Connor Feldman* Creating an Ontological System for a Digital Twin Building	*Daniel Delgado* Modeling Crystallographic Texture from Specific Pole Figures	*Myles Sherman* Characterization of Fluke 8588 for Digital Power Measurement
3:25 PM		*Daniel Coile* Predicting Fluid Properties of an Embedded Ink 3D Print Using Machine Learning	*Emily Buchanan* Utilization of Hyperpolarization in the Development of a Micro-MRI Imaging System
3:40 PM		*Ross Gunther* Maximizing Cell Viability in Embedded 3D Bioprinting	*Nicholas Entin* Developing Open-Source Hardware for Superconducting Single-Photon Detectors
3:55 PM			*Christopher Sherald* Modeling Devices for Atom-based Silicon Quantum Electronics
4:10 PM	Break		

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Wednesday, August 4, 2021 (4:20 to 6:05 PM (ET))

	NIST Center for Neutron Research (NCNR)	**Physical Measurement Lab (PML)**
	Moderator: Guebre X. Tessema (NSF Program Director)	**Moderator: Toni Litorja**
Time	Meeting Link: https://bluejeans.com/607919936/9168	Meeting Link: https://bluejeans.com/403818615/5811
4:20 PM	*Owen Bailey* Organic Cation Dynamics of Hybrid Vacancy-Ordered Perovskites $(FA)_2PtI_6$ and $(GA)_2PtI_6$	*William Barrett* Modulating the Optical Response of Multi-Resonant Nanostructures using Phase Change Materials
4:35 PM	*Kate Meuse* Classifying Spin-interactions using reinforcement learning	*Matthew Belzer* Assembly of Remote-Controlled Miniature LED Assembly
4:50 PM	*Jessica Opsahl-Ong* Optimizing neutron scattering measurements to best determine spin interactions in magnetic lattices	*Matthew Diaz* Simulating Charged Particle Energy Deposition
5:05 PM	*Patrick Park* Nuclear Design and Analysis of the NIST Replacement Reactor	*Ethan Swagel* Analysis of Complex Multidimensional Optical Spectra by Linear Prediction
5:20 PM		*Samuel Felsenfeld* Charged particle dynamics in a 0.7 T Unitary Penning Trap / Electron Beam Ion Trap
5:35 PM		*Nora Fayyazyddin Ljungberg* Optimizing detection probabilities of entangled photons
5:50 PM		*Ross Snyder* Creating a quantum toolbox for the web
6:05 PM	End of Day	End of Day

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Thursday, August 5, 2021 (10:00 to 12:00 PM (ET))

	NIST Center for Neutron Research (NCNR)	**Physical Measurement Lab (PML)**
	Moderator: Souleymane O. Diallo (National Facilities NSF Program Director)	**Moderator: Sujitra Pookpanratana**
Time	Meeting Link: https://bluejeans.com/607919936/9168	Meeting Link: https://bluejeans.com/403818615/5811
10:00 AM	[redacted]	*Henry Bell* Custom Calibration and Correction of Photoemission Electron Microscope Images
10:15 AM	[redacted]	*Dillion Cottrill* AlGaAs metalens for on-chip waveguide single-photon sources
10:30 AM	*Jack Rooks* Assessing Particle Orientation in Small Angle Neutron Scattering	*Alexander Loane* Calibration of Smart Grid Simulation Response to Oscillatory Waveforms
10:45 AM	*Daven Shah* Characterization of Spherical nanoparticles using Small-Angle X-ray Scattering as a Validation Metric for Neutron Interferometry	*Jacob Riddles* Simulating the Effects of XCT System Geometry Errors
11:00 AM	*Sydney Molnar* Optimizing a Magnetically Shielded Solenoid for Extended-Q SANS Polarization Analysis Capability	Break
11:15 AM	*Aurora Zemborain* Temperature-dependent binary solvent structure of solvent segregation driven gel (SeedGel)	*Ricardo Morales Sanchez* Resonator modeling for novel sound calibration technique
11:30 AM	*Ryan Puthumana* Investigating Lipid Bilayer Structures with Neutron Reflectometry	*Hoyean Le* Simulating the Simulator – A Computational Fluid Dynamic Analysis of NIST's Stack Simulator
11:45 AM	[redacted]	*Alessandro Rizzoni* Optimal Design of Fiber to Waveguide Facet Coupler Geometries Using the Finite Element Method
12:00 PM	Break	

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Thursday, August 5, 2021 (1:00 to 2:30 PM (ET))

	Physical Measurement Lab
	Moderator: Zachary Levine
Time	**Meeting Link:** **https://bluejeans.com/403818615/5811**
1:00 PM	*Molly Kreider* Modeling mode shifts in astro-etalons for high precision spectrographic calibration
1:15 PM	*Milan Richardson* Employing Machine Learning to Classify Bimolecular Translocation Events
1:30 PM	*Jared Schwartz* Branching Fractions and Oscillator Strengths in Singly Ionized Chromium
1:45 PM	*Cassie Stoffer* Investigating Temperature Changes in Low Field DNP
2:00 PM	*Catherine Silver* Optimization of Low and High pass Cutoff Parameters for Firearm Population Statistics
2:15 PM	*Daniel Bordwin* Assessing the causes of uncertainties within triaxial accelerometers
2:30 PM	Break

Summer Undergraduate Research Fellowship (SURF) Colloquium Parallel Session

Thursday, August 5, 2021 (3:00 to 5:00 PM (ET))

	Physical Measurement Lab
	Moderator: Gregory Cooksey
Time	**Meeting Link:** **https://bluejeans.com/403818615/5811**
3:00 PM	*Jason Hsu* Automated Collection and Control of Flow Cytometry on a Microchip
3:15 PM	*Nikita Podobedov* Graphical User Interface for Analysis of Data from a Serial Microfluidic Cytometer
3:30 PM	*Laura Zhou* Developing a unified statistical framework for the analysis of atomic clock data
3:45 PM	*Satvik Manjigani* Using Machine Learning to Characterize DNA Structures
4:15 PM	END
4:30 PM	
4:45 PM	
5:00 PM	

SURF Colloquium Session Links and Phone Numbers

- Plenary Session (August 3, 2021 at 10:00 AM to 12:00 PM (ET))
  Meeting Link: https://primetime.bluejeans.com/a2m/live-event/abyktxzj
  Join by phone:
  Dial one of the following numbers:
  +1 (415) 466-7000 (US) +1 (760) 699-0393 (US)
  PIN: 2313231 # PIN: 2205524472 #

- Parallel Session (August 3, 2021 to August 5, 2021 at 10:00 AM to 6:00 PM (ET))

  - **Communications Technology Laboratory (CTL)**
    Meeting Link: https://bluejeans.com/807706899/0663
    Phone:
    +1.202.795.3352 (United States (Washington DC))
    +1.408.317.9254 (US (San Jose))
    +1.888.748.9073 (United States (Primary))

    Meeting ID: 807 706 899
    Participant Passcode: 0663

  - **Engineering Laboratory (EL)**
    Meeting Link: https://bluejeans.com/455089596/4825
    Phone:
    +1.202.795.3352 (United States (Washington DC))
    +1.408.317.9254 (US (San Jose))
    +1.888.748.9073 (United States (Primary))

    Meeting ID: 455 089 596
    Participant Passcode: 4825

- **Information Technology Laboratory (ITL)**
  Meeting Link: https://bluejeans.com/649812750/4953
  Phone:
  +1.202.795.3352 (United States (Washington DC))
  +1.408.317.9254 (US (San Jose))
  +1.888.748.9073 (United States (Primary))

  Meeting ID: 649 812 750
  Participant Passcode: 4953

- **Material Measurement Laboratory (MML)**
  Meeting Link: https://bluejeans.com/471510305/3535
  Phone:
  +1.202.795.3352 (United States (Washington DC))
  +1.408.317.9254 (US (San Jose))
  +1.888.748.9073 (United States (Primary))

  Meeting ID: 471 510 305
  Participant Passcode: 3535

- **NIST Center for Neutron Research (NCNR)**
  Meeting Link: https://bluejeans.com/607919936/9168
  Phone:
  +1.202.795.3352 (United States (Washington DC))
  +1.408.317.9254 (US (San Jose))
  +1.888.748.9073 (United States (Primary))

  Meeting ID: 607 919 936
  Participant Passcode: 9168

- **Physical Measurement Laboratory (PML)**
  Meeting Link: https://bluejeans.com/403818615/5811
  Phone:
  +1.202.795.3352 (United States (Washington DC))
  +1.408.317.9254 (US (San Jose))
  +1.888.748.9073 (United States (Primary))

  Meeting ID: 403 818 615
  Participant Passcode: 5811

Communications Technology Laboratory (CTL) Participants

Sreyas Chacko

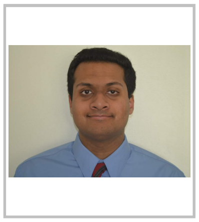
Megan Lizambri

Viktor Murray

Carolina Whitaker

Robert Xu

Marcus Zeender



SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name: Sreyas Sabu Chacko			
Academic Institution:	University of Maryland, College Park	**Major:**	Computer Science-Data Science Track
Academic Standing (Sept. 2021):	4th Year (Senior) Student		
Future Plans (School/Career):	Complete my undergraduate studies and seek a career in Data Science		
NIST Laboratory, Division, and Group:	CTL, Public Safety Communications Research, Mission Critical Voice Group		
NIST Research Advisor:	Jaden Pieper, Jesse Frey		
Title of Talk:	A study of the properties belonging to the Articulation Band Correlation Modified Rhyme Test		

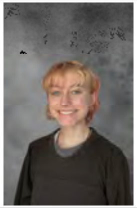
Abstract:

The Public Safety Communications Research Division (PSCR) of NIST works to help people working in public safety with their communication technologies. The Articulation Band Correlation Modified Rhyme Test (ABC-MRT16) is an algorithm which is used to estimate intelligibility of speech through a communication channel. Speech intelligibility is an important attribute because in high-risk situations, understanding communication could mean the difference between life and death. PSCR added a silence detector to ABC-MRT16 to address a perceived need to handle silent audio files. The silence detector uses a negative autocorrelation calculation from an audio file to determine if the audio file represents silence. Before the extensive study of the limits surrounding ABC-MRT16, the modifications needed for the improvement of the silence detector were unknown. In addition, verification was needed to see if the loudness of white gaussian noise would determine the response of ABC-MRT16 for the purposes of assessing the foundations of the algorithm.

Python code was used extensively for generating and calculating the results, and for one test, MATLAB was used to do the same. A csv file stored the results, which were subsequently extracted into JupyterLab for plotting and further calculations as needed.

Running these tests found that the silence detector suppressed pieces of audio which would have had a success value of 1. In addition, it was found that different volumes of white gaussian noise would yield a similar distribution regarding the variations of intelligibility which ABC-MRT16 claimed.

Based on those findings, it was concluded that the silence detector has properties which are too restrictive. Additionally, it was verified that when only white gaussian noise is analyzed by ABC-MRT16, volume does not matter.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Megan Lizambri

Academic Institution: University of Maryland, Baltimore County **Major:** Computer Engineering

Academic Standing (Sept. 2021): Sophomore

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

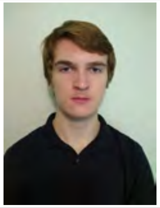
NIST Research Advisor: Evan Black

Title of Talk: NetSimulyzer - A 3D Network Simulation Analyzer for ns-3

Abstract:

Communications networks are extremely complex systems that require us to use computer simulation to understand how their components interact. A popular approach to simulation is to use discrete-event simulators such as ns-3, which is a free tool developed and maintained by the University of Washington ns-3 Consortium that is available under a GNU GPLv2 license. While ns-3 is powerful and supports simulating many types of networks, including wireless networks, it does not have a built-in capability for visualizing simulation outcomes. Also, the increased complexity of network protocols and scenarios is making the development, verification, and analysis of simulations a challenging task. To aid in those tasks, NIST developed NetSimulyzer, a flexible 3D visualizer for ns-3, to alleviate the workload of debugging, understanding, and demonstrating a simulated networking scenario. The tool easily integrates into any ns-3 scenario and provides core functionalities that are technology-agnostic. 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 new and improved 3D models for NetSimulyzer that we developed using an open-source, 3D modeling software tool, Blender, as well as a new feature, implemented in C++, that allows users to export collected data directly from the tool itself. By shaping and combining basic geometry and coloring surfaces, the new and improved models more closely resemble the real-world items that they represent, and they allow for additional information to be conveyed to the tool's users, while our improvements to the statistics component allow easier re-use of information and presentation of results. In conclusion, our work enables an enhanced user experience and further facilitates the development, verification, and analysis of simulations in ns-3.



SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name: Viktor Murray

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

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Work in industry as a backend or native developer.

NIST Laboratory, Division, and Group: CTL, Public Safety Communications Research, Mission Critical Voice

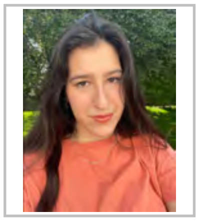
NIST Research Advisor: Jesse Frey

Title of Talk: Automated Unit Testing of Voice Quality of Experience Tools.

Abstract:

When first responders are working in the field, effective and reliable means of communication are essential for coordinating personnel. As part of their work to improve mission critical voice communication systems, the Public Safety Communications Research Division, Mission Critical Voice team has developed a set of Quality of Experience (QoE) software tools to measure and evaluate the performance and reliability of audio communications. These tools, written in Python, consist of a core library and associated plugins which must be installed individually in order to have the full functionality of the QoE system available. As a result, bugs or errors within the software may not be immediately visible when making changes due to their interdependent nature.

To facilitate future development and maintenance of these QoE tools, my project implements and improves automated unit testing for both the core library and plugins. Using Gitlab Continuous Integration/Deployment (CI/CD) these unit tests run automatically when the code is modified to verify that the code is still functional. The GitLab CI/CD workflow was set up to run tests for both the core library and plugins whenever a change is made to the library, but only run tests for the specific plugin when a plugin is changed. If a test fails, the granular nature of unit testing makes it trivial for the developer to determine the cause of any errors and correct them. This significantly reduces the workload for future developers maintaining the project and ensures accurate and reliable measurement systems for public safety communications.



SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name:	Carolina Whitaker		
Academic Institution:	Case Western Reserve University	**Major:**	Electrical & Computer Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Software Engineer		
NIST Laboratory, Division, and Group:	Public Safety Communications Research Division		
NIST Research Advisor:	Margaret Pinson and Scott Ledgerwood		
Title of Talk:	Image Quality for Computer Vision		

Abstract:

In computing, object detection algorithms are used to label a significant amount of common objects within a photo or a video. However, these algorithms are still relatively new and not fool proof, sometimes mislabeling or omitting objects humans would easily be able to detect in a piece of media. While some of these are failures of the algorithm, other problems stem from issues within the media itself (e.g. out of focus, grime on the lens, sun flare). By understanding the impact of camera impairments on computer vision algorithms, scientists can train computers to automatically assess the quality of images.

In this work, we look at a series of datasets submitted for a 2020 Public Safety Communication Research Division ’ s competition titled “ Enhancing Computer Vision for Public Safety Challenge ” . This challenge asked teams from across the country to submit a range of impaired images for further research in computer vision as well as pose possible failure metrics. After the winners were selected and announced, we took an initial look at the actual data presented to analyze what was given and find any errors, as well as clean the files. We also wanted to see if there was any merit to the metrics presented and use these ideas to compare commonly used object detection algorithms with one another to observe their behavior. So far, the analysis of the datasets and proposed metrics have shown that such algorithms do perform less accurately when media is impaired, as expected. Nevertheless, this project will be ongoing after this summer and will hopefully give some insight into understanding the failure rates of computer vision due to common camera impairments.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Robert Xu

Academic Institution: University of Notre Dame

Major: Electrical Engineering

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Commission as a United States naval officer in 2023. Hope to attend Nuclear Power School.

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

NIST Research Advisor: Dr. Peter Vouras

Title of Talk: Eliminate the Man-in-the-Middle: 5G Edge Security

Abstract:

The 5G cellular technology standard is a significant upgrade to current 4G network capabilities. Cellular networks have a ‘core’, which is a centralized network of high-capacity routing and switching equipment that sorts and processes data carried by the network, and an ‘edge’ that is made up of base stations – cell towers and antennas – that devices use to connect to the network. In 4G networks, the edge is mostly separate from the core. In 5G networks, significant processing power is moved from the core closer to the edge, and consequently, the entire network must be protected, with the edge and the core equally secure.

Narrowband phased array antennas are comprised of multiple individual antenna elements. They are equipped with a transmitter or receiver that phase-shifts incoming and outgoing signals. On transmit, the phase shifted signals interfere constructively in space to create a directional main beam, which allows devices to communicate over longer distances. This process is known as beamforming. In our project, we exploited destructive interference to create a quiet zone in the vicinity of an eavesdropper such that he lacks adequate received power to process the signal.

An example of a major threat to the 5G edge is the man-in-the-middle attack, in which an eavesdropper intercepts and alters communications between a base station and user. For this project, we wrote MATLAB scripts that demonstrate the effectiveness of electronic protection schemes against eavesdroppers. Our method precludes the initial entry of malicious signals into the network as opposed to software solutions that mitigate the threat after the fact. The simulation of base station and auxiliary phased arrays allow us to determine signal power at the eavesdropper’s location and the effectiveness of our signal cancellation technique, which depends on creating destructive interference in the direction of the eavesdropper. An advantage of our approach is that it works well with existing 4G or 5G base stations and does not require any expensive retrofits.

We first simulated the output of a 6 element by 6 element phased array at the base station, which radiates a sinusoidal signal at a frequency of 28 GHz. Using the distance between the base station and the eavesdropper, we calculated the received phase at the eavesdropper and coherently summed all the received signals from the base station. Next, we set up an auxiliary phased array located near the base station. We used it to transmit a signal that arrives at the eavesdropper equal in amplitude and 180 degrees out of phase with the signal received from the base station. These two signals cancel each other across the eavesdropper’s aperture. In fact, we observed a significant reduction in received signal power at the eavesdropper’s location; graphically, in the azimuth-elevation space, we observed deep nulls separated by a series of peaks. This distorted gain pattern should prevent the eavesdropper from demodulating and decoding the signal that we are trying to protect.

With this information, we hope to expand our simulation to incorporate more phased arrays and hardware so that we can generate data increasingly representative of a real operational environment.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name: Marckie Zeender

Academic Institution: Pomona College

Major: Physics

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate school or workforce

NIST Laboratory, Division, and Group: Mission Critical Voice, Public Safety Communications Reasearch, Quality of Experience

NIST Research Advisor: Jesse Frey, Jaden Pieper

Title of Talk: Mission Critical Voice Quality of Experience GUI

Abstract:

The Mission Critical Voice (MCV) team in the Public Safety Communications Research (PSCR) division is creating four quality of experience measurement systems to compare the legacy communication systems first responders currently use with new broadband systems. Setting up, configuring, and running the systems via a command-line interface is overly complex and onerous for the intended users; therefore, the goal of this project is to make the software user-friendly and to accentuate regularly used features against optional advanced features. This project organizes all four tests into one Graphical User Interface (GUI), using the python package tkinter. With just a few clicks of the mouse, the user may select a test, edit its parameters, log notes about it, and run it. While a test is running, the GUI reports on the test’s progress and estimates the time until completion. The GUI has key advantages for useability over the software’s command-line interface. Firstly, the GUI allows for more flexibility in setting and modifying the parameters, in contrast to entering the values manually every time. Secondly, the GUI guides the user through the required steps in an intuitive way and helps prevent mistakes in the configuration. This project hopes to provide a more accessible, convenient, and foolproof interface for MCV quality of experience tests.

Engineering Laboratory (EL) Participants

Cameron Busser

Donald Chang

Noelle Crump

Alex Dai

A’Di Dust

Conner Feldman

Samay Govani

Jonathon Gruener

Prasun Guragain

Divya Hadavale

Andrew Hoffpauir

Keely Hutchinson

Patrick James

Eugene Jeong

Yekta Kamali

Swathi Kashi

Sahil Kochar

Alex Kuan

Engineering Laboratory (EL) Participants (continued)

Aeron Liss

Reza Mirzaiee

Erik Mitchell

Isaac Park

Amaan Rahman

Nathan Rand

Dominique Regli

Lucia Rhode

Thomas Roche

Mary Ruxsarash

Derek Schoenberger

Michael Shao

Riya Sharma

Emily Shimabukuro

Mackenzie Smith

Bethany Taylor

Ashley Tisaranni

Matthew Weiss

Tyree Warren

Brian Woo-Shem

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Cameron Busser

Academic Institution: University Of Maryland, College Park **Major:** Psychology

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Attend Graduate School

NIST Laboratory, Division, and Group: Engineering Laboratory, Materials and Structural Systems Division, Emergency Communication Group

NIST Research Advisor: Dr. Emina Herovic

Title of Talk: Emergency Communication During Hurricane Maria

Abstract:

The landfall of Hurricane Maria in September 2017 caused immense destruction to Puerto Rico. It revealed the weaknesses within emergency communication systems as they failed in the midst of crisis. In order to understand the complexities within emergency communications and disaster response in Puerto Rico, the National Institute of Standards and Technology (NIST) commenced an extended research project intended to characterize the use of emergency communication and identify the factors that influenced the public's decision to take protective measures. Communication from before, during and after the storm was collected for analysis, resulting in thousands of official and unofficial statements, including news articles, Wireless Emergency Alerts, press releases, and social media posts. Qualitative Content Analysis will be conducted on emergency communication messages to assess their distribution and effectiveness. Deductive first level coding of news articles is conducted in line with the three core emergency preparedness perceptions defined by the Protective Action Decision Model. This process of categorization and coding will allow us to easily identify common themes within the emergency communication that influenced public response. The results from this project are projected to provide insight into how the emergency communication surrounding Hurricane Maria shaped the public's response to the emergency. This will help others understand the performance of emergency communications systems and thus lead to recommendations for improvement of communication standards. The investigation of emergency communication in Puerto Rico will not only exhibit the shortcomings of disaster response during Hurricane Maria, but also guide future emergency response efforts and aims to prevent such failure from occurring again.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Donald Chang		
Academic Institution:	University of Massachusetts Amherst	**Major:**	Mechanical Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Pursue a Master's in Mechanical Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Fire Research Division, WUI group		
NIST Research Advisor:	Shonali Nazare		
Title of Talk:	A Review of Heat Flux Measurements in Large Wildland Experiments		

Abstract:

The wildland urban interface (WUI) setting, where residential structures and communities are constructed next to natural fuels, is particularly at risk for fire spread. Guidelines for prevention and mitigation of fire spread in wildland urban interface settings should be backed up by reliable data both from WUI and wildland fire experiments. Robust heat flux measurements are critical for scientists to determine fire behaviors in large wildland experiments, but problems with instrumentation and assessing different heat flux mechanisms presents challenges. Past large wildland experiments have obtained preliminary results on measurements to characterize fires, but these experiments face similar challenges that is not yet elucidated to a wider audience.

The approach to address measurement and instrumentation issues is to review literature on large-scale wildland experiments and document information on instrumentation, peak heat flux and temperature values, the uncertainty associated with measurements, limitations, advantages, as well as operating principles of devices used, and necessary background information. Several papers on structural fires, and wildland fire experiments have been reviewed and analyzed. Typical values reported in literature are gas temperatures ranging from 600°C-1300°C and total heat fluxes up to 300kW/m^2. Generally, an uncertainty of 3% is reported for all measurements. The review of literature indicates Gardon gages, thin skin calorimeters, and type K thermocouples are generally used, both, in wildland and WUI related fire experiments. Current instrumentation lacks the ability to quantify heat fluxes at high temporal and spatial resolution over larger scales. Recent research suggests sensible heat flux measurements and flow fields derived from coincident nadir radar and infrared measurements can address the spatial and temporal issues. Attempts to quantify heat fluxes over large scale experiments has emphasized the importance of remotely sensed measurements and deepen our understanding of fire energy transport processes in wildland fires.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Noelle Crump			
Academic Institution:	Worcester Polytechnic Institute	**Major:**	Mechanical Engineering
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Finish Bachelors Degree in Mechanical Engineering		
NIST Laboratory, Division, and Group:	Engineering Labratory, Fire Reaserch Division, Engineered Fire Saftey Group		
NIST Research Advisor:	Randal McDermott		
Title of Talk:	Modeling Windflow Over Large-scale Complex Geometries		

Abstract:

Computational Fluid Dynamics models are promising tools in fire safety. The National Institute of Standards and Technology (NIST) has developed a Fire Dynamics Simulator (FDS) software for this purpose.

The Fire Dynamics Simulator uses dynamics, geometrical obstructions, and initial boundary conditions to model wind velocity and temperature within the simulation area. To ensure the accuracy of the simulation, identical test cases are run in the computer simulation and in the lab, and the results of the two are compared. For accurate simulation results, cases must be run at suitable resolution and with appropriate geometrical obstructions. For large-scale, high-resolution cases, a computing cluster must be used.

The goal of this project was to record data from a model of wind flowing over Askervein Hill and compare it to data collected and described in the Askervein Hill Project Research Report. The simulation was conducted over a computational area much larger than a room or house and utilized the Fire Dynamics Simulator's complex geometry capabilities to model the hill with an array of vertices and faces rather than a collection of cubes. The wind in the model can be simulated using the mean windspeed and direction over Askervein Hill recorded from the report, and the behavior of the atmospheric boundary layer is modeled using the Monin-Obukhov similarity theory.

The case was run on the Fire Research Division's Blaze and Burn computing clusters, and data was collected from virtual devices set to measure specific quantities from within the simulation at the specific locations the anemometers were placed on the Hill as described in the report. The results were then plotted with the results from the Askervein Report.

The results from this study will help provide insight to the accuracy of the Fire Dynamics Simulator's complex geometry capabilities and will serve as valuable data for the validity of future simulations.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Alex Dai

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

Academic Standing (Sept. 2021): Sophomore Year

Future Plans (School/Career): I plan on completing my undergraduate degree, then finding a stable job hopefully close to my home.

NIST Laboratory, Division, and Group: Engineering Laboratory, Systems Integration Division, Information Modeling & Testing Group

NIST Research Advisor: Thurston Sexton

Title of Talk: Continuous Integration for Collaborative Web Documentation: Updating the AI-COI Catalog

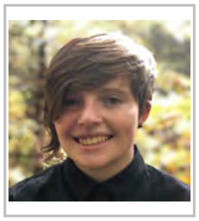
Abstract:

The NIST Artificial Intelligence Community of Interest (AI-COI) has maintained a catalog of AI-related projects in NIST laboratories for several years. As the quantity and variety of projects increases, providing a scalable mechanism to collaboratively maintain the catalog will be key to its longevity.

Because the catalog is volunteer-supported, a key issue in maintaining it arises from ensuring the information listed for each project gets validated. We developed a system using the Python programming language, in combination with human-readable project metadata, to automate significant amounts of the needed validation process. Through a script, we can now validate a document using a list of key values (such as keywords, contributors, project title, etc). These can be continuously tested as part of an automated pipeline using NIST's GitLab instance, reducing the need for manual review by volunteers going forward.

Another need for the catalog is to ensure easy access by NIST staff. The catalog has been loaded to an internal webpage that can be searched for useful information, or aggregated for insights. The metadata system described above can be used—with templates we created—to provide automated, consistent formatting of project pages, reducing volunteer effort and enabling flexible changes to the catalog going forward, as needed.

If successful, this effort may provide a template for similar efforts across NIST to follow. This process and techniques we developed can be replicated in other catalogs or documentation efforts with relatively minor changes. All source code has been made available to NIST staff via GitLab.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	A'di Dust		
Academic Institution:	Macalester College	**Major:**	Computer Science
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Pursue a PhD with research in the area of machine learning and intelligent robotics		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent Systems Division, Cognition and Collaboration Systems Group		
NIST Research Advisor:	William Harrison		
Title of Talk:	Generalized Procedural Generation With Measured Alteration For Robot Agility		

Abstract:

Intelligent industrial robots need a variety of diverse environments to train in. An agile robot needs to be able to repeat a task in a dynamic environment. If reinforcement learning is being used for training a robot model, the robot model learns specifically from the environments it is exposed to, meaning that more diverse environments should make the robot more agile. There also needs to be measurements of the amount the environment is being altered to make non-anecdotal observations about the effect of environment alteration on robotic performance. Precise measurement could give insight into the types of environments in which the intelligent robot succeeds and the types in which it struggles. The goal for this project was to design an algorithm that generates diverse environments based on specifications, while also providing a means to compare robot agility.

To implement this algorithm, the 3D gaming engine, Unity and 3D industrial objects were used. The result of this research is software to create industrial robot testing environments and measure the alterations made to different aspects of the environments. The designer inputs parameters specific to their needs, such as which parts are used and where obstacles for the robot might be. The software then outputs 3D environments. Each 3D environment has a score that measures the amount of alteration of the parts used by the robots and the obstacles in the path of the robot. These alterations include varying the orientation, spacing, and number of parts and obstacles. Each 3D environment also has a score that measures the amount of alteration of the environment's inside and outside lighting.

This project allows for industrial robot designers to precisely measure the agility of their robot while generalizing the environment generation process and maximizing the level of environment diversity.

SURF Student Colloquium

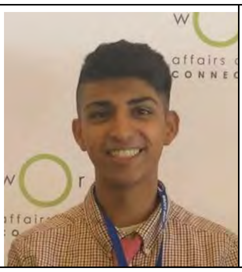
NIST – Gaithersburg, MD August
2-6, 2021

Name:	Connor Feldman
Academic Institution:	Hamilton College
Major:	Physics
Academic Standing (Sept. 2021):	Senior
Future Plans (School/Career):	Unsure
NIST Laboratory, Division, and Group:	Engineering Laboratory, Division 732, Group 2
NIST Research Advisor:	Parastoo Delgoshaei
Title of Talk:	Creating an Ontological System for a Digital Twin Building

Abstract:

In combination with the Department of Energy, the NIST Engineering Laboratory is currently developing a semantic model that will be used as standardization for commercial Heating, Ventilating, and Air Conditioning (HVAC) systems. The purpose of this model is to integrate data from heterogenous sources related to buildings. This model will monitor the system, locate devices and segments that need to be repaired, and allow for more cost-effective and energy efficient use of heating and cooling systems. The model uses artificial intelligence, so users can enter basic information about components and the model can infer complicated relationships between components.

Using this semantic model, which is still being developed, we mapped out a model of the HVAC system that exists in the NIST Intelligent Building Agents Laboratory (IBAL). We input relationships between equipment in the lab into the model and then asked the model competency questions (queried the model) that are crucial for applications such as fault detection and diagnostics, commissioning, and energy auditing. This exercise will help determine shortcomings of the standard model and test the user-friendliness of the querying interface. This standard semantic model will be an essential component of Digital Twins for buildings.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Samay Govani

Academic Institution: Worcester Polytechnic Institute

Major: Robotics and Mechanical Engineering

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): completing undergraduate degree program and working in industry

NIST Laboratory, Division, and Group: Engineering Lab, Intelligent Systems Division, Signals & Perception Systems

NIST Research Advisor: Shelly Bagchi & Jennifer Case

Title of Talk:
Interfaces for Human-Robot Interaction

Abstract:

Soft Robotics is a promising new field within robotics, focused on systems composed of soft sensors, actuators, compliant structures, etc. Due to the flexibility and adaptability of soft robots, common applications include surgical robots, exosuits or rehabilitation devices, and exploratory robots. This project's focus is continuum robots, which are heavily inspired by biological systems such as elephant trunks and octopus tentacles. In this project, we concentrate on cable-driven continuum robots, wherein tension placed on cables running through the length of the robot creates movement. While there are models describing the behavior of continuum robots, there are no easy-to-use design tools to assist with cable placement that would enable new users to easily enter the field and participate in system design. At the National Institute of Standards and Technology, a model of a cable-driven continuum robot was created in MATLAB that requires multiple complex inputs: matrices dealing with the placement of cables within sections of the robots which are entered into the model using command-line inputs. In this project, a comprehensive GUI (Graphical User Interface) was designed to remove the model from command-line input. Ultimately making the interface more accessible and usable by individuals with little knowledge of soft robots or programming.

In an industrial factory setting, testing new machines and planning out the motion paths of autonomous machines can be an arduous task, requiring physically placing the robot in the location and manually programming the robot, requiring experience generally not present in the factory. At NIST, using models of common industrial robots, an application has been developed in Unity wherein the 3D image of a UR5 industrial robot arm appears and its end effector can be guided using a target point on the screen via dragging or clicking. In this project, additional user interface items were added to incorporate learning or teaching by demonstration to the UR5 Unity model. The user can input multiple points on the screen via dragging a target around or inputting coordinates, and the robot will navigate to the points in order. Using learning from demonstration principles, the robot then can be prompted to maneuver to the target points in a specific order. This feature enables teaching by demonstration in the interface, target points can be added or taken out. Thus, the user can graphically program operations such as pick-and-place via our interface with no experience in programming.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Jonathon Gruener

Academic Institution: University of Colorado Boulder **Major:** Mechanical Engineering

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Pursue a graduate degree

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

NIST Research Advisor: Dr. David Goodwin

Title of Talk: Development of tracking software for fiber-reinforced polymer composite and concrete samples

Abstract:

Buildings, bridges, and other structures often can develop structural weaknesses as they grow older and the building materials are exposed to the elements, such as concrete. As concrete deteriorates or requires strengthening to handle additional loads, retrofitting with fiber-reinforced polymer composites is one solution. The use of fiber-reinforced polymers has grown significantly in the past 20 years but there further research is needed for unified design, inspection, or maintenance specifications to ensure uniformity and stability of the products, especially outdoors. The NIST project discussed here was designed to gain an understanding of fiber-reinforced polymer performance outdoors to aid in the development of design and inspection procedures.

Representative samples of fiber-reinforced polymer composites will be sent to weathering fields across various climates in the United States. A tracking system was needed to help tag and categorize these samples and streamline the data collection process. Furthermore, the tag was needed to track the location and testing status of the samples. Near-Field Communication tags were chosen as the most effective way to physically tie data to a specific sample. A Google Form link was loaded onto each tag and opens upon interaction with the tag. The form is used to collect data about the sample. The form then transfers the input to a database stored on NIST servers. A similar Near-Field Communications system was implemented in the collection of evidence from the Champlain Towers collapse in Florida during this internship.

Since outdoor weathering of FRP specimens is anticipated to last for more than five years, a reliable system was needed to effectively catalogue the samples. The software will store the dates of sample deployment and testing data for each sample. This allows clear and organized data storage as well as easy exporting to graphing or analysis software. The software was written with modularity in mind, to allow easy transitioning to new systems or editors.

The program was written in Python to allow for the logging of each unique sample as well as the dates and times the samples arrived and left the weather fields. A reminder system was created to assist in the timely return of samples to NIST. Additionally, a user interface was built to allow the bulk viewing of samples at a given site and to give a snapshot of the progress of the entire project.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Prasun Guragain

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

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): I plan to attend graduate school

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

NIST Research Advisor: Allison Barnard Feeney

Title of Talk: Web-based software for investigating and evaluating data tampering

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 Systems Engineering Group at NIST is creating a software solution that allows any level of the supply chain to examine the distribution of tampered data using model-based integration techniques, such as data mapping, which is the process of matching fields from one data source to another. The group is developing a cybersecurity awareness software focused on data tampering issues, driven by security controls and activities defined in the NIST Cybersecurity Framework and NIST SP 800-53. The software will streamline communication between the users and a cybersecurity team about any unusual activities in the business. We are adding the capability:

- for users to report the incidents to warn the cybersecurity team
- for users to track their incident tickets
- for the cybersecurity team to manage and respond to incident tickets

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Divya Hadavale			
Academic Institution:	Clovis Community College	**Major:**	Biology
Academic Standing (Sept. 2021):	Sophomore		
Future Plans (School/Career):	University of California, Irvine		
NIST Laboratory, Division, and Group:	Engineering Laboratory		
NIST Research Advisor:	Jennifer Helgeson		
Title of Talk:	Impacts of Complex Events		

Abstract:

There is recognition that complex events tend to create impact that is greater than the sum of its parts. These complex events include hurricanes and COVID-19 impacts. Furthermore, it is possible that complex events make individuals, institutions, and communities more vulnerable to future events. In this project, GIS assessment is being used to note trends, such as assessing “hot spots” of complex events including natural hazards and COVID-19 and also aim to look at a policy meant to address one event (COVID-19), while there are other contributing factors that may not be considered in the provision of support. This project involves performing analysis on the socio-economic impacts related to the distribution of COVID recovery funding. Specific tasks include data cleaning and gathering of specific datasets in preparation for analysis (statistical, geospatial, or a combination of the two). In doing so, datasets are combined based on specific geographic identification codes, exploratory analysis is performed on the combined datasets, and the findings are presented in the form of a series of numeric and graphical representations.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Andrew Hoffpauir

Academic Institution:	University of Louisiana at Lafayette	**Major:**	Mechanical Engineering

Academic Standing (Sept. 2021):	Graduate Student at the University of Virginia
Future Plans (School/Career):	Attend graduate School at the University of Virginia to pursue a Master's in Biomedical Engineering
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligence Systems Division, Manipulation and Mobility Systems Group
NIST Research Advisor:	Kenny Kimble
Title of Talk:	A Biofidelic Impact Dummy to Evaluate the Safety of Collaborative Robot Applications

Abstract:

Collaborative robots are used in many workplaces to increase the efficiency and competitiveness of manufacturing. Determining the safety of these collaborative robots in the workplace is important to ensure users will not gain injuries from interacting with them. ISO/TS 15066 provides a list of biomechanical limits on force and pressure for various body parts in case of human-robot impact. Developing a test dummy that mimics the mass properties, mechanics, and anthropometry of the human body is necessary to validate the safety of these collaborative robots in the workplace. The test dummy design should be repeatable, easy to manufacture, easy to set up, easy to use, easy to calibrate, and minimize cost.

An accurate model of a 50th percentile male, determined by the US National Highway Traffic Safety Administration (NHTSA) THOR automotive crash dummy is leveraged for the design of the test device. Sensors, including a soft force capacitive sensor, still in development, will be placed in the dummy components at points marked from the Fraunhofer IFF human subject force/displacement test data to validate the properties of the test dummy. Force testing will be completed to validate the safety of the interactions between the robot and dummy body to ensure it is safe to use in the workplace. A forearm has been developed and validated that proves the design features and fabrication process of the test device. The forearm will guide the development of an upper arm component that will eventually be incorporated into a full right arm assembly with the end goal of a completed full-body dummy.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Keely Hutchinson

Academic Institution: Kansas State University

Major: Mechanical Engineering

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate Studies

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

NIST Research Advisor: Dr. Ho Yeung

Title of Talk: Improvements in Laser-Powder-Bed-Fusion Additive Manufacturing Using Open-Platform Software

Abstract:

Additive manufacturing (AM) technology has evolved from its early use in preproduction prototyping to being used regularly to fabricate parts used in the aerospace, medical, automotive, and many other industries. One type of AM process is laser powder bed fusion (LPBF), in which a laser is used on metal powder to selectively fuse cross-sections of the intended model into a thin layer of metal. This process is repeated after each successive layer of metal powder is spread across the completed layer. At the National Institute of Standards and Technology (NIST) the Additive Manufacturing Metrology Testbed (AMMT), a fully custom and open-platform system, is being used to perform research on the LPBF process. The principal goals of this research are optimizing the LPBF process and creating high-quality repeatable parts. Simple Additive Manufacturing (SAM) software is an open-platform AM preparation software developed for use with the NIST AMMT. SAM slices a 3D model into layers, fills the layers with scan paths, creates G-code to describe the scan path, and interprets the G-code path into digital commands to drive the testbed. My research during the Summer Undergraduate Research Fellowship (SURF) program focuses on the research and development of this open-platform AM preparation software.

My research goals for the summer are to review literature on and become familiar with LPBF additive manufacturing, to test, and write a user manual for, the SAM software. I continue to review literature from NIST and other publications on LPBF AM. I am testing the SAM software, while noting where future changes and improvements to the software could be implemented. I also study the scan strategies implemented on commercial AM machines, and recreate them with SAM for comparison. I am writing, editing, and organizing a user manual to document the SAM software, and intend to include figures and examples to add clarity for the reader.

SURF Student Colloquium

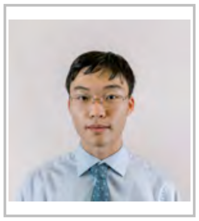
NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Patrick James		
Academic Institution:	University of Maryland at College Park	**Major:**	Mechanical Engineering
Academic Standing (Sept. 2021):	Sophomore		
Future Plans (School/Career):	Finish my undergraduate degree and then enter graduate school		
NIST Laboratory, Division, and Group:	Engineering Lab, Materials and Structural Systems Division, Earthquake Engineering Group		
NIST Research Advisor:	Dr. Jazalyn Dukes		
Title of Talk:	Analysis of Key Wall Characteristics in FRP Retrofitted Shear Wall Database		

Abstract:

Fiber reinforced polymers (FRP) have been used to strengthen walls in old buildings in order to make them more resistant to earthquakes. Many of these older buildings are not up to current code standards. In some areas this may not be a major problem but in other areas such as Florida or California, this can be a major problem especially when dealing with either sub-standard buildings or high seismic activity. FRP retrofits greatly increase the load capacity of walls, most often reinforced concrete (RC) walls. A database of experiments on FRP retrofitted shear walls was developed by NIST to gain insight into real world applications and improve understanding of these components to improve the use in the field.

This summer, my project consists of three parts related to the shear wall database. The first part is digitizing and constructing the backbone curves from existing force-displacement hysteretic curves. The second part is identifying the key parameters that influence the response of a wall by reviewing existing literature and graphing the parameters against the drift ratio in Microsoft Excel. Finally, the third part of my project will culminate in a recommendation for testing. This will help fill in gaps in the current database which will be used to make recommendations to update current building codes.



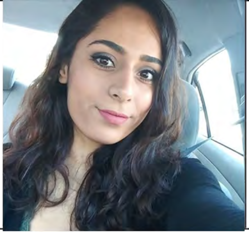
SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Eugene Jeong		
Academic Institution:	Cornell University	**Major:**	Mechanical Engineering
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Master of Engineering Program		
NIST Laboratory, Division, and Group:	Engineering Laboratory		
NIST Research Advisor:	Dr. Jason Fox		
Title of Talk:	Comparison of Segmentation Methods for an Additively Manufactured Surface		

Abstract:

Measuring surface texture is critical to evaluate the accuracy of a workpiece and the process that created it. Characterizing a surface involves calculation of parameters, and for areal data, also includes segmentation into regions containing three dimensional features of interest. For laser powder bed fusion, a type of additive manufacturing, such features include partially melted powder and spatter particles that appear on the surface of the workpiece. These particles contribute to the finish of a part and to its applications, for example, in heat transfer where surface area is important. A number of algorithms exist for segmenting features from surface data, and one has been standardized in ISO 25178-2. Since every algorithm produces different boundaries, better understanding the performance of segmentation algorithms would be valuable for future study of manufactured surfaces. In this project, three methods of segmentation were chosen to analyze height data for an additively manufactured surface: thresholding by gradient, contour stability, and watershed with combination. Additionally, the data was preprocessed with various Gaussian and sharp-cutoff filters. Each of the methods (filtering plus segmentation) were compared for accuracy in identifying feature points compared to a manually masked reference, by calculating scoring parameters on a feature-wise and full-area basis. The performance of each method indicates its usability for identifying particles on a nominally flat surface with waviness and form present. A full description of the filtering, segmentation, and scoring algorithms is presented.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Yekta Kamali		
Academic Institution:	University of Maryland College Park	**Major:**	Electrical Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Graduating May 2022 and then applying for a Master's. Pursue a career in engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Intelligent System Division, Cognition and Collaboration Systems Group		
NIST Research Advisor:	Brian A. Weiss		
Title of Talk:	Performance Analysis of a Position Verification Sensor for Robot Workcell Health Degradation Assessment		

Abstract:

Over the last few decades, robotic technology has dramatically advanced. Humans continue to leverage robots to perform challenging, repetitive, or unsafe tasks. Robots improve production efficiency, as robots are capable of doing repetitive, unsafe, or high precision tasks. To further production efficiency, robots should be built such that they are accurate to minimize the potential for mistakes.
The manufacturing research team I am a part of developed a Position Verification Sensor (PVS) to test the repeatability of a robot workcell's accuracy. The sensor's precision is adjustable and currently tests a robot's precision up to 0.001". The project employs a multi-axis linear stage to verify the sensor's performance, separate from the robot workcell.

Instead of manually checking hundreds of points, the verification test has been automated. The automated multi-axis stage is controlled by a laptop running MATLAB script that instructs the stage where to move. The script picks points either randomly, horizontally, or vertically and then simulates robot movement with an attempt to insert the key into the PVS. An Oscilloscope connected to the PVS' digital output determines the success of each attempted insertion. This feedback is integrated into MATLAB and the output is captured into Excel.

A method is constructed that accepts multiple data sets and fuses them into a single analysis and percentage table that displays the overall findings for each position. Color-laden heatmaps and tables display the results. An initial goal is to color-code the analysis and percentage tables to provide an "easy to understand" visual to the analysis consumer. A follow-on goal is developing a MATLAB script to determine the sensor's boundary conditions by eliminating locations that we know will 100% pass or fail.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Swathi Kashi

Academic Institution: Illinois Institute of Technology

Major: Mechanical Engineering

Academic Standing (Sept. 2021): Graduate Student

Future Plans (School/Career): I plan to graduate from the Illinois Institute of Technology with a Bachelors in Mechanical Engineering and a Masters in Materials Science and Engineering.

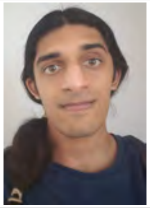
NIST Laboratory, Division, and Group: Engineering Lab, Materials and Structural Systems Division, Earthquake Engineering Group

NIST Research Advisor: Matthew Speicher

Title of Talk: Energy-based Seismic Assessment Criteria

Abstract:

Following the 1994 earthquake in Northridge, California, changes were made to the way that buildings' seismic performances were evaluated. There were new standards established for constructing buildings and for evaluating already existing buildings. For the latter specifically, the American Society of Civil Engineers (ASCE) 41 Standards was developed. ASCE 41 establishes performance-based design standards for structural components and connections of already existing buildings and its current acceptance criteria is based on a component's maximum deformation, which is a result of its loading history. While this is an effective method for evaluating performance, it is possible that there are other ways to predict a component's seismic performance without considering its loading history. The main goal of this project was to determine if that possibility is true. Experimental data, specifically geometry, strength, and energy dissipation measurements of various specimens under various loading protocols were collected and Energy [kN-m] was normalized by dividing it by Yield Strength [kPa]. Then, various combinations of parameters were plotted against Normalized Energy Dissipation to determine if a lower bound value could be established that was independent of load history. For one component, Wide-Flange Beams, under the American Institute of Steel Construction (AISC) loading protocol, the product of web slenderness, flange slenderness, and length-to-radius-of-gyration ratios divided by axial load was plotted. While there was an initial decrease in energy, the data stayed consistently between 0.0008 meters cubed and 0.0015 meters cubed after a certain value of geometric parameters over axial load was reached, suggesting that for certain ranges of the geometry to axial load ratio, a critical lower bound value may be obtainable. Once similar plots are developed for other loading protocols, a comparison of results will be done to determine if this lower bound is valid, and if the hypothesis can be confirmed.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Sahil Kochar

Academic Institution: University of Maryland - College Park

Major: Aerospace Engineering & Mathematics

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Graduate School, Likely in Aerospace Engineering

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

NIST Research Advisor: Dr. Xiaohong Gu

Title of Talk: Web-based Tool for Service Life Prediction of Photovoltaics and Building Materials

Abstract:

There is rapid growth in the use and study of Photovoltaic (PV) systems to provide clean, renewable energy. These systems come with polymeric encapsulation materials, which are susceptible to degradation under ultraviolet (UV) light, heat, moisture, and other environmental stresses, leading to shortened service lives. In order to estimate the service life of a given PV system, it is necessary to perform tests on the component polymers. However, testing in real world conditions is prohibitively time-consuming, so accelerated indoor testing is necessary to achieve a reasonable development time for new PV products.

This testing involves irradiating the material with many times more UV radiation than it would receive outdoors, performing the tests at high temperature to accelerate the degradation reactions, and altering the relative humidity as that affects certain reactions. Matching these accelerated tests to real world conditions is not trivial, and requires very sensitive estimations of activation energy and other parameters of the degradation reactions. As the range of polymers used for these purposes is so varied, these parameters cannot generally be determined analytically and must be estimated from testing.

The web tool in this project — developed in R Shiny for its data science features — does just that, fitting parameters according to a degradation model developed primarily at NIST. After performing their own tests, PV developers may upload their test data to the tool to determine these parameters and examine how well the model fits their data — from both accelerated indoor tests and real-world outdoor tests. The model can function with only degradation and total irradiance measurements, and allows for refinement with the addition of irradiance spectrum, temperature, and/or relative humidity data. Validating the model on their data will give the confidence to make accurate predictions on the service life of their products.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Alexander Kuan

Academic Institution: University of Maryland, Baltimore County **Major:** Information Systems

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Finish my undergraduate degree and then either work or continue into graduate school

NIST Laboratory, Division, and Group: Engineering Laboratory, System Integration Division, Information Technology and Testing Group

NIST Research Advisor: Yan Lu

Title of Talk: Data Curation Tool Development and In-Situ Monitoring Data Analysis for Additive Manufacturing

Abstract:

Additive Manufacturing (AM) enables the production of comprehensive 3D models based on a 3D digital design; however, the creation of these features is texturally inconsistent with each consecutive build of an identical part. The procurement of data has a critical role to play in the in-situ monitoring of the development of each model throughout its AM lifecycle. Utilizing metadata specifications, image data is recorded on each layer during the entire process of the build to use for various AM product studies. This project aims to investigate the status of the AM data collection and enhance the Additive Manufacturing Materials Database (AMMD) software functions to display recently curated AM data more effectively.

This project focuses on curating, analyzing, and visualizing the in-situ and ex-situ data generated from powder-bed-fusion AM processes. The Overhang Part X4 study showcases four parts with 250 burned layers using the same build metadata and XYPT commands. Post-build X-ray computed tomography (XCT) data related to the study demonstrate the noticeable differences of a surface cleaned model compared to the pre-built 3D model design, though layer images captured by the in-situ process monitoring do not match the number of TIF images of the XCT data.

The tasks of this project include curating data for the Overhang Part X4 in-situ and enhancing XCT data visualization software for the AMMD. Once implemented, an algorithm is developed using OpenCV and MATLAB to register the XCT stack images against the layerwise images predicted from in-process monitoring. In other words, the XCT images stacked at 12 micron voxel size must be aligned to the in-process data at a layer thickness of 20 micron. Syncing the different sets of images will simplify the search of the right images on the data visualization tool and enable the correlation between in-process data and XCT images.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Aeron Liss		
Academic Institution:	Shippensburg University	**Major:**	Advanced Physics
Academic Standing (Sept. 2021):	Recent graduate from SU		
Future Plans (School/Career):	I plan to aquire more research/similar work experiences then attend grad school.		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Building Energy and Environment Division, Heat Transfer and Alternative Energy Systems Group		
NIST Research Advisor:	Dr. Brianna Conrad		
Title of Talk:	Photovoltaic Cell Processing and Calibration Using Electroluminescence Hyperspectral Imaging Measurements		

Abstract:

Solar photovoltaic cells, which convert light into electricity, are used in a wide variety of ways, ranging from running handheld calculators, to utility-scale power plants capable of powering a small town. Accurate characterization of solar photovoltaic devices is important because it allows one to determine device performance, understand factors affecting performance, as well as characterize properties of device materials. The information and understanding gained from characterization can lead to improvements in device performance. Electroluminescence (EL) hyperspectral imaging is a powerful characterization tool that lets us see spatially resolved performance information. The hyperspectral imager records spectrally resolved luminescence images in absolute values with arbitrary units, which the calibration process uses to get an absolute photon emission rate. The previous method of characterization used proprietary software that only produced an absolute photon emission rate averaged over the entire cell. I developed a method using a mathematical programming environment to efficiently manipulate large data files, and generate calibrated absolute hyperspectral images while making full use of the data collected. This method can be used to determine spatially resolved values important to understanding photovoltaic performance, such as pseudo-IV curves, and external luminescence efficiency. This can be further used to examine the influence of various types of defective regions with cells. This approach allows the calibration process to be expanded to incorporate new analysis techniques as they are developed.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Reza Manuel Mirzaiee

Academic Institution: University of Virginia **Major:** Computer Science

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Work in-industry for graphics applications.

NIST Laboratory, Division, and Group: Engineering Lab, Systems Integration Divison, Extended Digital Thread

NIST Research Advisor: William Bernstein

Title of Talk: Retargetable Animations for Indrustrial Augmented Reality

Abstract:

Due to its tremendous potential, Industrial Augmented Reality (AR) has experienced a recent surge in adoption and integration within the manufacturing enterprise. However, the maintenance cost of updating animations due to upstream changes or client-specific design variations is very expensive. Currently, platform-agnostic standards for Computer-Aided Design (CAD) files provide precise definitions for geometry and functionality, but do not specify kinematic animations in their entirety. Hence, in practice, animations need to be individually updated or re-tooled manually. This work showcases a method for implementing geometry-independent AR assembly animations onto three dimensional CAD files using simple skeletal armatures, a technique widely used in the gaming and entertainment industries. This technique allows for upstream engineering design changes to propagate through to the AR assembly visualization. Through this harmonization of standards, we may achieve a more automated pipeline for handling animations in industrial AR systems, leading to better interoperability, maintainability, and flexibility.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Erik Mitchell		
Academic Institution:	Santa Clara University	**Major:**	Computer Science and Engineering
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Pursuing an M.S. in Computer Science and Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Smart Grid Program Office		
NIST Research Advisor:	Thomas Roth		
Title of Talk:	Prediction of Energy Consumption in Residential Homes using a Reinforcement Learning Algorithm		

Abstract:

Renewable energy sources such as solar photovoltaic (PV) have become an important part of the residential energy market. The consumption and production of energy is more dynamic as more residential homes are becoming producers of energy and this energy source is dependent on weather conditions. The increased adoption of renewables in the residential sector requires a new strategy for managing the power grid to ensure reliability.

In order to balance supply and demand of energy, a dynamic energy pricing model is needed to optimize energy consumption. In such a system, homes are incentivized to prioritize energy use when it's cheaper such as during times when energy demand is lower (non-peak times) or when local energy production is higher (PV production during the day). In heating, ventilation, and air conditioning (HVAC) systems, this means utilizing preheating and precooling in order to lower energy costs while maintaining comfort levels. At the same time, electric utilities need to know the energy needs of each home in order to balance the system. As such, there is a need for a robust method to predict energy consumption for grid operation.

In this project, a machine learning algorithm is used to predict the energy consumption of a residential HVAC system given data on the temperature inside the home, the surrounding weather, and the market price of energy. Optimization has also been built into the algorithm, discouraging energy use and encouraging precooling and preheating while maintaining temperature comfort levels. The reinforcement learning algorithm was integrated with a building simulator called EnergyPlus, containing the house model and temperature conditions, to produce the results. The simulations were done using a co-simulation platform called the Universal CPS Environment for Federation (UCEF) from NIST.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Isaac Park

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

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate School in Machine Learning

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

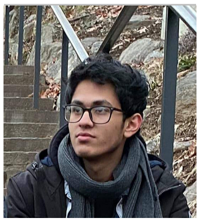
NIST Research Advisor: Marcos Vanella

Title of Talk: Beta Testing Unstructured Geometry within FDS using Pyrosim

Abstract:

The Fire Dynamics Simulator (FDS) was developed by the Fire Research Division at NIST as a computational fluid dynamics (CFD) model of fire-driven fluid flow. Within FDS obstacles can be defined using grid conforming obstructions or, lately, unstructured geometries. As part of the current FDS development and release cycle, the use of unstructured geometries is being tested and validated to ensure accuracy and reliability.

In the present work, the user workflow for fire scenario definition using unstructured geometry models is developed and evaluated. Several obstacles and compartments of increasing complexity are defined in Autodesk Inventor and then imported into the commercial FDS preprocessor Pyrosim. Pyrosim provides a simple way for users to develop FDS input files and work with FDS models. For the new unstructured geometry, we test components of Pyrosim to ensure the correct translation of details from its graphical user interface to FDS input files. The cases developed correspond to validation test compartments, from a single test section to multiple-room houses, and provide the opportunity to test the calculations with respect to experimental data. Along the beta testing process, we have found and addressed several issues related to model preparation, FDS functionality, and simulation capabilities.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Amaan Rahman

Academic Institution: The Cooper Union **Major:** Electrical Engineering

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate with BE in Electrical Engineering and Masters of Engineering; pursue PhD in either pure mathematics or neural networks

NIST Laboratory, Division, and Group: Engineering Laboratory; Intelligent Systems Division; Manipulation and Mobility Systems Group

NIST Research Advisor: Li-Baboud, Ya-Shian; Virts, Ann; Shah, Mili

Title of Talk: Markerless Human Kinematic and Kinetic Evaluation with 3D Monocular Pose Estimation Algorithms

Abstract:

Evaluation of exoskeleton performance analysis introduces standards for exoskeletons to ensure proper functionality and safety for the subject. Currently, there are limited standard evaluation methods for exoskeletons. Methods that are under investigation by the NIST Exoskeletons and Exosuits Research and Standard Test Methods team are applications of Optical Tracking System (OTS), markerless pose estimation methods, and Inertial Measurement Units (IMUs) to analyze exoskeleton user kinematics and to infer kinetic information to understand the impact of exoskeletons on a subject's joint movement and forces. This project focuses on investigating markerless 3D pose estimation algorithms to determine their viability as methods for tracking human joint position and deriving skeletal frame orientations.

3D pose estimation applies a Convolutional Neural Network (CNN) structure to estimate the 3D pose and joints of individual(s). 3D monocular pose estimation algorithms are investigated to measure error between the estimated 3D pose and ground truth data (OTS and IMU data) by examining human limb orientations and joint positions. Current methods under investigation: Graph Attention Spatio-Temporal Convolution Network (GAST-NET), Video Inference for Human Body Pose and Shape Estimation (VIBE), and 3D Multi-Person Pose Estimation (3D-MPPE). The project consisted of evaluating the algorithms on videos of gait and hurdle tests; the hurdle test had additional challenges of limb occlusion.

The calculation of error metrics, Percent Detected Joints (PDJ) and Mean Per Joint Position Error (MPJPE), between various 3D monocular pose estimation algorithms and ground truth data provide a proper standard to determine precision and accuracy of pose estimation algorithms. Stereo based algorithms yielded MPJPE values between 10 mm to 50 mm and monocular based algorithms yielded MPJPE values between 30 mm to 90 mm. However, stereophotogrammetry requires synchronized cameras and calibration data, whereas most monovision algorithms do not. Spatio-Temporal models such as GAST-NET yield MPJPE values as low as 30 mm; through visual inspection, the algorithm detected joint positions even with occlusions by the hurdle test apparatus. The initial algorithm evaluation demonstrated the method was a strong candidate for markerless 3D joint detection and position estimation.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Nathan Rand

Academic Institution: Virginia Tech **Major:** Aerospace Engineering

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Attend graduate school and then either enter industry or pursue a PhD (primarily focusing on propulsion technology).

NIST Laboratory, Division, and Group: Engineering Laboratory, Divison 735

NIST Research Advisor: Dr. Deisenroth

Title of Talk: Data Specification for AM Machine Performance Tests

Abstract:

Metal additive manufacturing, specifically laser powder bed fusion, provides a revolutionary approach to the manufacturing of metal parts; however, this approach has struggled to gain widespread implementation despite all its benefits. Manufacturing techniques that have gained more widespread implementation than metal laser powder bed fusion have benefitted from the development of standard performance data formats that have resulted in broadly accepted test data frameworks, which have not yet been achieved for laser powder bed fusion. Here we used an XML Schema to delineate a framework for laser powder bed fusion machine performance data and its related metadata fields. The fields were divided into generic and specific test categories and implemented based on in-depth research into previous tests and documentation, along with existing data standards for other manufacturing techniques. Furthermore, the XML Schema was designed with an emphasis on flexibility and ease of use to facilitate successful application to various performance tests, as well as to facilitate test reproducibility by a variety of machine users. Integration of a Python XML conversion tool was investigated to ensure that the resulting framework could be readily applied by industrial and academic users. This seminal research on the development of a standard performance data format for laser powder bed fusion is a step toward broader acceptance of this manufacturing technique for the production of high-quality and custom metal parts that will have lasting impacts on projects ranging from human space flight to customized medical prosthetics.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Dominique Regli

Academic Institution: The Johns Hopkins University

Major: Engineering Mechanics

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Pursue a career in industry before attending graduate school

NIST Laboratory, Division, and Group: Engineering Laboratory, Division 735

NIST Research Advisor: Gregory W. Vogl, Ph.D.

Title of Talk: Cutting Force Monitoring for Smart Machine Tools

Abstract:

Machine tools are vital to the production of milled precision parts worldwide. The spindle within these machines is the rotating element that enables the cutting process. When working properly, the cutting forces generated between the rotating tool in the spindle and the material being milled yield a relatively smooth and accurate part surface. However, prolonged use of these spindles causes degradation of the spindle and the cutting tools, ultimately resulting in poor production quality and unplanned downtime for the machines. Ideally, part errors and cutting forces could be predicted through spindle monitoring, but the current methods for machine health management are not cost effective for major manufacturers. A fast, data rich, and inexpensive solution is needed to monitor the real-time performance of machine tools.

In this project, we take a new approach to spindle health tracking designed for efficiency and accuracy. A spindle testbed measures magnetic "cutting" forces and on-machine accelerations while a custom tool holder spins. The goal of this project was to create a model that relates the on-machine accelerations to the cutting forces, so that when applied to actual machine tool data, the measured accelerations can be used to estimate the cutting forces. To achieve this goal, Fourier transforms of the data were used to set up a least-squares solution within MATLAB, which yields an equation of motion (a model) that dictates the movement experienced by the spindle. Various models were compared based on metrics (e.g., the root mean square error) to determine how close the estimated forces from each model are to the measured forces. With these relationships known, the real-time accelerometer signals were then inputted into the model to estimate the real-time "cutting" forces. The estimated forces agreed fairly well to the measured forces. Thus, this process of data collection and model development could be implemented within machine tools to monitor cutting processes and improve quality control in real-time manufacturing.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

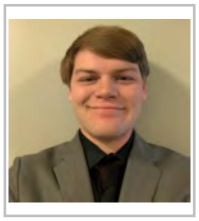
Name: Lucia Rhode			
Academic Institution:	The Cooper Union	**Major:**	Electrical Engineering
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Engineering Laboratory; Intelligent Systems Division; Manipulation and Mobility Systems Group		
NIST Research Advisor:	Ya-Shian Li-Baboud, Mili Shah, Ann Virts		
Title of Talk:	Annotated Dataset for Exoskeleton Pose Estimation and Fit Evaluation		

Abstract:

Exoskeletons are wearable robots meant to work with the human body to help improve performance and alleviate pressure from strenuous movements. Exoskeletons have potential in the healthcare field and in industry and manufacturing. The fit of an exoskeleton is important as an ill-fitted exoskeleton may cause pain or harm to the user.

NIST is researching the effect of exoskeletons on movement to develop exoskeleton standards. A goal as part of this research is to create a marker-less vision-based system using pose estimation to track key-points of the user and the exoskeleton and develop metrics to evaluate the fit of the exoskeleton. The purpose of this project is to build an annotated dataset to inform the pose estimation algorithm.

The dataset is based on image data collected for the development and evaluation of exoskeleton safety and performance test methods. The studies include knee bends and simulated peg-in-hole industrial tasks. Traditionally, a training set would have to be annotated by hand. This is costly and time consuming. DeepLabCut is a toolbox that is pre-trained on a robust pose-estimation model and allows the user to track user-defined key points with minimal hand annotated frames. An annotation guide was developed to keep annotations consistent and gather input from biometric experts and exoskeleton engineers. Annotations will be validated visually and quantitatively. Validation frames will be manually annotated and compared to the annotations by DeepLabCut by obtaining the 2D pixel positions and determining the Euclidean distance. Initial annotated videos using DeepLabCut show promising visual results and illuminate initial fit evaluation metrics.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Thomas William Roche		
Academic Institution:	University of Maryland, College Park	**Major:**	Fire Protection Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Continue education to a Masters and PhD in Fire Protection Engineering		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Division 730, Applied Economics Office		
NIST Research Advisor:	Juan Fung		
Title of Talk:	Buyout Programs for Community Resilience		

Abstract:

Voluntary Buyout Programs have been popular risk management policies for river and coastal cities experiencing flooding disasters for the past few decades. The buyout program offers to purchase damaged properties within the flood zone to convert them into either greenspaces or new buildings. A buyout program was utilized after the 2008 Cedar Rapids flood to both assist the homeowners of the damaged properties and reinvest funding into the city. This research tracks the homeowners who were eligible for the buyout program determine where they moved and how beneficial the program was in terms of post-buyout property value.

Data from property records for 2007-2016 was standardized in order to match property owner names across properties and time. The standardized property data was combined with spatial data on flood impact to determine buyout eligibility, as well as data on the buyout program, to determine buyout recipients. Exploratory analysis with the standardized data provided demographic information on the economic status of properties across the study period. Initial results indicate that property owners who accepted the buyout program (especially those in residential units) were economically worse off than their non-buyout counterparts, with approximately 75% of buyout recipients being given less money than their house was worth in 2007, and about 50% of non-buyout properties retained or exceeded their 2007 value. This research will determine how these rates apply to property owners who owned both buyout and non-buyout properties, as well as where people moved post-buyout.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Mary Ruxsarash

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

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Pursue Graduate School and PhD

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

NIST Research Advisor: Dr. Stephanie Watson

Title of Talk: Statistical Analysis of Condition Monitoring Test Data from Accelerated Aged Nuclear Power Plant Electrical Cables

Abstract:

As of 2020, Nuclear Power Plants have been the provider for about 20% of the U.S's electricity. Electrical cables used in these plants are vital to the function and safety of the overall operation. However, these cables are also subject to degradation due to varying levels of humidity, radiation and temperature. Due to large quantities and limited access, replacing cables is an expensive and time consuming task. Condition Monitoring Tests (CMTs) and aging management programs have recently been used in the nuclear industry to evaluate changes in mechanical, electrical and chemical properties of cables throughout their service lives. These tests aim to determine the proper time which cables have degraded and must be replaced.

This project's overall goal is to evaluate the effectiveness of commonly used CMT's such as Elongation at Break (EAB), Oxidation Induction Time (OIT) and Thermogravimetric Analysis (TGA) to track electrical cable degradation. To simulate accelerated operational aging, NIST conducted a 16-month aging experiment at Sandia National Laboratory's Gamma Irradiation Facility. Cables were aged in novel environmental chambers of varying temperatures, levels of humidity and radiation dose
Cable specimens were removed at 2-month intervals and subject to various CMT's. For this summer project, We've approached interpreting the resulting CMT data from six test methods for the entire 8 aging interval period that were analyzed using various statistical and analytical methods. The data collected offers a valuable glimpse into which CMT's efficiently track aging and if mechanical, electrical and chemical properties measurably change with respect to various conditions of aging.

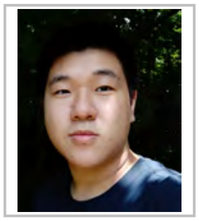
SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Derek Schoenberger		
Academic Institution:	University of Maryland, College Park	**Major:**	Mechanical Engineering, Computer Sci.
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Pursuing a career as a design engineer doing R&D in the energy, transportation, or robotics sectors		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Life Cycle Engineering Group		
NIST Research Advisor:	Guodong Shao		
Title of Talk:	A Case Study of Modeling Machine Tool Systems using Standards		

Abstract:

Following the demand for a system neutral solution for exchanging Computer-aided (CAX) model information, the international standard ISO10303 (also known as Standard Exchange of Product Data (STEP)) was developed. While most CAX tools allow users to represent and transfer geometric information in STEP format, kinematic information is not accounted for in STEP models exported from CAX systems. This presents major challenges in the exchange, analysis, and simulation of Computer Numerical Control (CNC) machining systems that include complex kinematics. A solution to this is to represent fully assembled machine tool models in a neutral file format, such as STEP, with both geometric and kinematic information included. Currently, to accomplish this, an interface application needs to be developed to support the conversion of kinematic information from the CAX model to the STEP format. This study proposes the development of such an application that extracts kinematic information from a machine model in a vendor-specific format (e.g., Creo in this case) and constructs the information using the STEP standard so both geometric and kinematic information can be automatically generated. A CAX tool (PTC Creo Parametric) and two open-source STEP related tools (JSDAI and STEPutils) are used to support the application development. Java, J-link, and Python are required to use these tools. Using the aforementioned methods and tools, a preliminary prototype application has been developed to demonstrate the viability of this kinematic data exchange approach. The same approach can be used to develop a fully functional application or applications for different CAX tools to automatically convert kinematic information of CAX models. By representing fully assembled machine models in a neutral file format such as STEP, machine models with complex kinematics can be accurately and efficiently exchanged and evaluated on any CAX proprietary tool. The development of the application proposed in this project will support the ease of exchanging information across CAX platforms and help reduce the time spent refactoring kinematic models.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Michael Shao		
Academic Institution:	University of California, San Diego	**Major:**	Computer Engineering
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Participate in research and internship programs to better inform my decision on graduate school		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Materials and Structural Systems, Disaster Statutory Programs		
NIST Research Advisor:	Tanya Brown-Giammanco		
Title of Talk:	Better Hurricane Preparedness and Recovery through Data Analysis and Predictive Algorithms		

Abstract:

The National Institute of Standards and Technology (NIST) uses a Decision Criteria score sheet developed for the National Construction Safety Team (NCST) to evaluate the impact of hurricanes and other disaster events. Traditionally, this evaluation requires someone to manually review publicly available data, social and traditional media, such as weather reports, emails, and communication with local authorities, to measure/judge the damage.

Our group set out to define concrete criteria for the effect of Hurricanes (as opposed to human judgment) to implement a program that predicts the scores on the Decision Criteria score sheet before landfall in order to automate the scoring process, streamline hurricane response preparations, and to lessen the effect of bias in the scoring process.

The program, hosted on John Hopkins University's SciServer platform, pulls the latest forecast data from the National Hurricane Center (NHC) along with population and Social Vulnerability Index (SVI) ratings to quickly estimate the affected population and level of impact along the forecast track of the hurricane. Using these data, the program generates a predicted score for the Decision Criteria score sheet.

We ran this program on various datasets of previous hurricanes, most notably Hurricane Michael, over the 2021 Summer. The results are then compared to previous, manually created scores, so we can evaluate the accuracy of our model and refine how we evaluate the relevant metrics.

Our process will speed up hurricane event preparation, response and recovery process and help standardize they way we evaluate the impact of hurricanes.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Riya Sharma

Academic Institution: University of Maryland College Park

Major: Mechanical Engineering and Anthropology

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate School, Research, Energy/Sustainability, Humanitarian Engineering

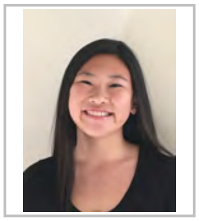
NIST Laboratory, Division, and Group: Engineering Laboratory, Division 731, Hurricane Maria Group

NIST Research Advisor: Dr. Emina Herovic

Title of Talk: Emergency Communication During Hurricane Maria

Abstract:

The landfall of Hurricane Maria in September 2017 caused immense destruction to Puerto Rico. It revealed the weaknesses within emergency communication systems as they failed in the midst of crisis. In order to understand the complexities within emergency communications and disaster response in Puerto Rico, the National Institute of Standards and Technology (NIST) commenced an extended research project intended to characterize the use of emergency communication and identify the factors that influenced the public's decision to take protective measures. Communication from before, during and after the storm was collected for analysis, resulting in 7,386 texts including official and unofficial statements, news updates, and social media posts. Qualitative Content Analysis will be conducted on emergency communications and messages to assess their distribution and effectiveness. Deductive first level coding is conducted in line with the three core emergency preparedness perceptions defined by the Protective Action Decision Model. Deductive second level coding focuses on how the aforementioned core perceptions are in part influenced by the media frames described by Framing Theory. As the analysis process progresses, we will determine inductive framing codes as necessary. This process of categorization and coding will make accessing information much easier for future work. After completing the Qualitative Content Analysis and coding all excerpts, a report will be written to communicate findings. The research from this project will help others understand the performance of emergency communications systems and the public's response to these communications. The investigation of emergency communication in Puerto Rico will not only exhibit the shortcomings of disaster response during Hurricane Maria, but also guide future emergency response efforts and aims to prevent such failure from occurring again.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Emily Shimabukuro		
Academic Institution:	Oberlin College	**Major:**	Engineering
Academic Standing (Sept. 2021):	Sophomore		
Future Plans (School/Career):	Chemical Engineer		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Systems Integration Division, Systems Engineering		
NIST Research Advisor:	Evan Wallace		
Title of Talk:	Visualization of Traceability Data		

Abstract:

In order to comply with the Food Safety and Modernization Act (FSMA), records must be kept of critical tracking events as food moves through the supply chain. These records aid in tracing the source of contamination to the origin in the event of an outbreak of foodborne illness. These same records will be used to quickly identify other affected products, so they can be recalled. These critical tracking events (CTEs) are events that are important in a product's history and can be grouped into categories based on the type of event-- movement, transformation, possession change, observation, or maintenance. These CTEs were chosen because it is both necessary information, and for the most part, records that organizations already keep. The latter part is imperative because companies need the collection of information to take as little time and additional effort as possible.

Graphs can be used to visualize this data, as these records in their raw form are too massive for a person to easily and quickly understand. In the case of an outbreak, the speed of traceability is of utmost importance. So, graphs called ontologies are used as a schema to visualize the data by connecting related data points and allowing for easy tracing forward and backward. These graphs are good because they are easily read, and can be followed through each stage of production.

In collaboration with Texas State University, and companies like Land O'Lakes, this group has developed ontologies modeling the movement of grain through the supply chain. Using query languages like SPARQL to find records stored in RDF format (Resource Description Framework), one can navigate through the database, as well as find information about the grain as it moves and goes through stages of production.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Mackenzie Smith

Academic Institution: University at Buffalo **Major:** Biomedical Engineering

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): I plan to have a career in industry, potentially going to graduate school after a few years of work.

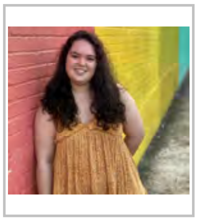
NIST Laboratory, Division, and Group: Engineering Laboratory, Materials and Structural Systems Division, Infrastructure Materials Group

NIST Research Advisor: Aron Newman, PhD

Title of Talk: Using X-ray Diffraction to Predict Cement Expansion From Sulfate Attack

Abstract:

When cement comes into contact with a sulfate solution, a chemical reaction ensues, resulting in the cement softening, cracking, and expanding in volume. In regions with high levels of sulfate in the soil and water, this reaction threatens the integrity of building foundations, bridges, and other infrastructure. Cemer samples can be tested for their susceptibility to sulfate expansion through ASTM International standardized tests, but these generally take 6 to 12 months to complete; meanwhile, obtaining the X-ray diffraction (XRD) pattern for a cement sample is approximated a one hour measurement. As such, using the XRD pattern and the peak intensities at numerous 2-theta values to predict a cement sample's propensity for sulfate expansion would save both time and money. We tested different machine learning algorithms to see which model could most accurately predict the percent expansion of 18 different kinds o cement, both in bulk and chemically-treated form. First, we utilized principal component analysis to reduce the number of predictive variables from almost 2800 different 2-theta values to three linear combinations. We then tested seven different regression models, and we found the mean-squared error of linear regression to be lower than both the other models and the variance of the percent expansion values for our samples. Having a mean-squared error less than the variance of the expansion indicates that our model significantly aids in the prediction of a cement sample's sulfate expansion, and it can be used to predict the general susceptibility to sulfate attack. Utilizing this model can aid manufacturers in selecting more durable kinds of cement for their construction projects.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Bethany Taylor		
Academic Institution:	University of Maryland	**Major:**	Mechanical Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Work and attend graduate school part time		
NIST Laboratory, Division, and Group:	Engineering Laboratory, Energy and Environment Division, Mechanical Systems and Controls Group		
NIST Research Advisor:	Natascha Milesi-Ferretti and Mike Galler		
Title of Talk:	Semi-automated Building Commissioning using HVAC-Cx		

Abstract:

Commercial buildings account for 40% of the total energy used in America. Buildings on average waste about 30% of the energy they use and the Heating, Ventilation, and Air Conditioning (HVAC) systems account for a significant amount of that wasted energy. Normally, commissioning of a commercial building would be very labor intensive and is not financially motivating. HVAC- Cx is a semi-automated building commissioning software tool developed by NIST that analyzes the performance of the HVAC system for ongoing monitoring and functional performance testing. In this project, the ongoing monitoring capability is used to detect faults determined by expert rules to generate fault reports and present the data on graphs. The HVAC-Cx aims to improve the system performance for occupancy comfort, energy management and equipment life. This project uses HVAC-Cx to analyze data collected from the Performing Arts Center at Montgomery College on the Rockville campus. Data collected from February to July of 2021 has been analyzed for faults and potential causes and presented to the building facility's staff. Faults are determined by the expert rules such as a common Fault 4 seen throughout this time period. During heating mode, the heating coils signal it is full open which indicates the system could be out of control. Many causes can be responsible for this such as the supply air temperature, mixed air and return air sensor not working properly. During different occupied modes such as heating or cooling the system has different faults with different causes from sensor malfunction to control sequence logic faults.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Ashley Tisaranni

Academic Institution: Florida Institute of Technology **Major:** Aerospace Engineering

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Rocket Scientist and Aspiring Astronaut

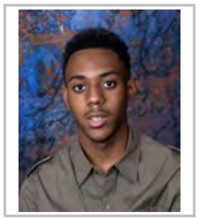
NIST Laboratory, Division, and Group: Engineering Laboratory, Intelligent Systems Division, Cognition and Calibration Studies Group

NIST Research Advisor: Pavel Piliptchak

Title of Talk: Artificial Intelligence for Manufacturing Robotics

Abstract:

Artificial intelligent (AI) robotics in the manufacturing industry is critical to the advancement of production innovation. The majority of modern robots in manufacturing are hard coded with specific functions and abilities, limiting the tasks that they are able to perform. Machine learning (ML) algorithms enable robots to learn by developing systems of neurons to interpret scenarios and execute intricate and individualized tasks. There are many forms of research, studies, and tests currently in progress within the industry to implement AI into manufacturing, but the field is missing established standards and resources to bring together the separate AI and manufacturing communities. Research is being conducted by NIST to reveal the possible future impact of industrial AI robots. The information is showcased in an “AI for Manufacturing Robotics Initiative” website serving as an easily accessible and understandable overview of how AI can be used in manufacturing. The website includes many recommendations and alternate sources for more detailed information. This project focuses on informing the research community about AI for manufacturing using a series of overview pages and a case study. The overview pages were developed using HTML to explain the evolution of ML algorithms and how they are implemented to allow robots to execute tasks. The case study involved training a robotic grasping maneuver method on a NIST dataset. This work contributes to informing the public through the website about AI for manufacturing robotics and its benefits to the industry.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Tyree Warren

Academic Institution: University of Maryland College Park **Major:** Aerospace Engineering

Academic Standing (Sept. 2021): Good Standing

Future Plans (School/Career): After graduating I hope to become an Aerospace Engineer

NIST Laboratory, Division, and Group: Engineering Laboratory
735.13

NIST Research Advisor: John Michaloski

Title of Talk: Peg in Hole Assembly

Abstract:

Peg in hole assembly is the most common task for manipulators to go through during any manufacturing process. In the most basic sense the task involves inserting an object into a hole, similar to a plug into an outlet. The goal of my research was to enable me to find patterns in previous works to create/simulate the best robot to accomplish the task. Then improving upon past works to specifically benefit small businesses. Due to COVD-19 I was unable to enter the lab, but I was able to simulate the scenario using by learning ROS and Gazebo. I also was able to learn Python, Linux, and Git. All while doing research on other Robot assembly algorithms. After learning I took information from those who have accomplished the task and trying to innovate by combining bits and pieces from each product. During my research I consistently saw similar designs. For example replicating human features (hands and arms) to onto a robot and having the robot mimic human behavior. Almost all of the designs used force and torque sensors to replicate the human sense of touch, however some used cameras and visual automation to mimic our sense of sight. Throughout my research I found that the most common structure of the robot mimics our fingers. The Most common devices are F/T sensors that enable the robot to find the hole. Finally, Small businesses are unable to afford high end equipment that many cutting edge robots use, and should stay away from vision guided peg in hole assembly robots. Also humanoid robots with unnecessary features.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Matthew Weiss

Academic Institution: University of Maryland-College Park

Major: Mechanical Engineering

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Attend Graduate School

NIST Laboratory, Division, and Group: Engineering Laboratory, Intelligent Systems Division, Manipulation and Mobility Systems

NIST Research Advisor: Vinh Nguyen

Title of Talk: Multi-Robot Control Through CRPI Interface

Abstract:

Robotic systems are becoming more complex and sophisticated in both their functionality and capabilities. This has lead to improvements allowing multiple robots working together on any given task. However, controlling a system of robots while they accomplish their tasks can be a complex process requiring multiple interfaces, which significantly increases the complexities and execution of any given procedure.

In an effort to create a universal interface for robot collaboration, the NIST ISD team has developed a collaborative robot programming interface (CRPI). The current version of CRPI utilizes the C++ programing language to interact with the various robots. However, to make the program more accessible to the general public, the program is being converted into the programing language Python. The development of the code from C++ to Python has been undertaken through the use of several different softwares; including Microsoft Visual Studio, PyCharm, and pybind11. The C++ code is accessed through Microsoft Visual Studio where it is formated such that the pybind11 software can convert it into Python modules. Once this is done, the Python module can be tested with PyCharm to see if the converted module is able to interface with the robots successfully.

Already, a library of C++ code has been translated into Python and shows the capacity to run as a Python module. This would indicate that it is possible to convert the entirety of the C++ code into Python modules. Through the use of Python based modules, the general public will be able to more easily interface with CRPI.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Brian Woo-Shem

Academic Institution: Santa Clara University **Major:** Mechanical Engineering

Academic Standing (Sept. 2021): Incoming Graduate Student

Future Plans (School/Career): Graduate school, then career as a mechanical engineer.

NIST Laboratory, Division, and Group: Engineering Laboratory, 730/Headquarters, Smart Grid and Cyber-Physical Systems Program Office

NIST Research Advisor: Thomas Roth, Cuong Nguyen

Title of Talk: Occupancy-Based Heating & Cooling Control to Increase Residential Energy Efficiency

Abstract:

Air conditioning use is expected to more than double worldwide by 2040 because of increased access to electricity, population growth, and climate change. Adding Heating, Ventilation and Air Conditioning (HVAC) can increase energy consumption by over 25 %, threatening to overwhelm the electric grid and complicating the transition away from fossil fuels. Better HVAC efficiency through methods such as operating only when buildings are occupied can offset the impact of additional houses with HVAC. This project develops a strategy for using predicted occupancy and current occupancy information in a home HVAC controller to reduce electricity costs while maintaining comfortable temperatures. The occupancy controller builds on recent innovations in thermostat efficiency, including a controller that adapts to weather while helping balance the supply versus demand of electricity, and non-invasive occupancy detection using widely available sensors.

Occupancy adjustments save energy by reducing or shutting off HVAC when nobody is inside, but cannot cause discomfort when residents are home. The controller uses occupancy detection to identify when people are present and maintain comfortable temperatures. Probability of occupancy guides operating HVAC in preparation for arrival, reducing the odds that a resident returns to an uncomfortable temperature house. To validate this occupancy-based temperature algorithm, simulations were performed using the Universal CPS Environment for Federation (UCEF) platform developed by NIST to link the EnergyPlus building energy simulator with different controllers. HVAC energy consumption for conventional and occupancy optimized thermostats in a model residence were compared. Preliminary results indicate that the optimized controller decreases energy cost compared to traditional thermostats, while maintaining a comfortable temperature for occupants nearly all of the time. This occupancy-based thermostat works in tandem with weather adaptation, time of use optimization, and electric consumption coordination improvements to increase efficiency and ease the burden of HVAC on the electric grid.

Information Technology Laboratory (ITL) Participants

Isabel Agnostino

Nina Agrawal

Nizar Benmohamed

Robert Bennet

John Bodenschatz

Marc Burlina

Khar Casse

Justen Chen

Elizabeth Euwart

Jason Eveleth

Nishaant Goswamy

Muktaka Joshipura

Raymond Karyshyn

Sophie Koh

John Kucera

Peter Lef

Denis Liu

Information Technology Laboratory (ITL) Participants (continued)

Elvin Liu

Matteo Marchi

Lindsay Marean

Connor Mooney

Erchis Patwardhan

Karol Sadek

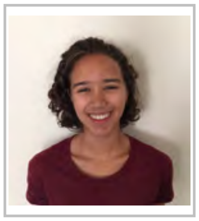
Dominique Regli

Peter Shin

Ramon Suris-Rodriguez

Selena Xiao

Joshua Zarb



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Isabel Agostino			
Academic Institution:	William & Mary	**Major:**	Applied Mathematics
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	I plan to have a career in operations research.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics		
NIST Research Advisor:	Michael Mascagni		
Title of Talk:	Star-Discrepancy		

Abstract:

High-level financial calculations often utilize quasi-Monte Carlo methods instead of their truly random counterparts due to the properties of more uniformly distributed point sets. One such measure of uniformity in quasi-random sets is the star-discrepancy, the supremum of local discrepancies which compare the volume of an s-dimensional space within the [0,1)^s unit cube to the proportion of the set's points within said space. In high dimensions, calculating star-discrepancy for quasi-Monte Carlo point sets is an NP-hard problem. Since star-discrepancy represents a maximum of the local discrepancy function, mathematicians are now exploring optimization techniques such as random walks, genetic algorithms, simulated annealing, and machine learning, to approximate the star-discrepancy. To evaluate the performance of such algorithms, well-known point sets with known star-discrepancies must be generated and utilized. The Halton and Sobol sequences are two of the most famous sequences used to generate quasi-random point sets; thus, star-discrepancy for point sets of various sizes and dimensions from both the Halton and Sobol sequences have been calculated. If an approximation method for star-discrepancy is found to be significantly accurate, ease and cost of calculating star-discrepancy will be greatly improved.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Nina Agrawal

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

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Graduate School, hope to get master's degree in artificial intelligence

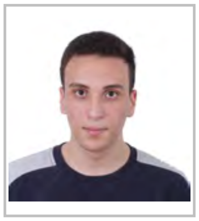
NIST Laboratory, Division, and Group: Information Technology Laboratory,Division 775, Information Systems Group

NIST Research Advisor: Derek Juba

Title of Talk: Identifying Carbon Nanotubes Using Machine Learning

Abstract:

ZENO software, developed by researchers at the National Institutes of Standards and Technology (NIST), computes a material's properties from the shape of its particles. Our objective is to perform what ZENO does in reverse; we wish to identify a material when provided with its properties. Our chosen material was carbon nanotubes as they are commonly used at NIST and can easily be generated using VMD software. In addition, carbon nanotubes can easily be identified by their length and chirality vectors. We developed a data set consisting of about 1620 nanotubes and loaded their properties into WEKA machine learning software. We then added random errors to the properties, up to 1%, to simulate experimental error. Using WEKA, we employed several supervised machine learning algorithms to estimate the lengths of the nanotubes as well as the angles of the chirality vectors for the data with errors as well as without. The algorithms we used were Linear Regression, Simple Linear Regression, Multilayer Perceptron, and Support Vector Regression. For each algorithm, we used WEKA to find the root mean square error (RMSE) of the predictions based on eight properties. We then further filtered the properties to ones that are experimentally measurable and ran the algorithms specified above on each property individually. Based on our data, we anticipate that machine learning can be used to invert the ZENO algorithm and use a nanotube's properties to predict its structure. However, further information is needed to draw exact conclusions.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Nizar Benmohamed
Academic Institution:	UMBC
Major:	Computer Science
Academic Standing (Sept. 2021):	Sophomore
Future Plans (School/Career):	Graduate School
NIST Laboratory, Division, and Group:	ITL, Software and Systems Division, Information Systems Group
NIST Research Advisor:	Timothy Blattner
Title of Talk:	High Performance Python

Abstract:

Python is a high-level programming language and is often found to be one of the easiest programming languages to learn and use thanks to its simplicity. However, this simplicity comes at a cost to performance. Python is an interpreted language and parallelization is often done through multi-process execution. One methodology to improve python's performance is through external, highly optimized python libraries that contain bindings into more high-performance languages, such as C++. C++ has mechanisms to obtain performance, such as multi-threaded parallelism and vector instructions. Unlike python, C++ is a compiled language, meaning that a C++ program can be compiled and optimized for a target system architecture.

In order to both utilize the simplicity of Python and the high performance of C++, we propose to analyze a variety of C++ to Python bindings that can make C++ code callable from Python. In this research we study, 3 such wrappers: Cython, PyBind11, and SWIG. These wrappers generate CPython files that contain C modules that are callable from Python.

Our target application is a high performance multi-threaded image loading library that streams partial areas of an image for processing, called FastLoader. We will explore the use of this data streaming approach and how it can be utilized in python while also trying to understand its performance impacts. The three wrappers offer a variety of capabilities, such as simplicity for creating bindings, mechanisms to release the Global Interpreter Lock (GIL), and tools to provide portability. We will compare and contrast these approaches and identify recommendations for creating these bindings. Lastly, we analyze the performance by using existing python libraries on the data that we pass from our bindings to compute statistics on high resolution images. This will be compared with a baseline approach that uses Python's ImageIO library, doing the same computation.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Robert Bennett

Academic Institution: Bloomsburg University of Pennsylvania **Major:** Mathematics

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate School- PhD Biostatistics

NIST Laboratory, Division, and Group: Information Technology Lab (ITL), Div. 775 Software and Systems, Information Systems Group

NIST Research Advisor: Joe Chalfoun, Adele Peskin

Title of Talk: Analysis of Biomedical Image Segmentations - Low-Field MRI

Abstract:

Low-Field Magnetic Resonance Imaging has the potential to introduce comprehensive diagnostic imaging in many scenarios where it is not currently feasible. These images are not always conducive to accurate diagnoses, due to low spatial resolution and noise. To overcome the challenges of low signal-to-noise ratio in these images, benchmarks are established using a diffusion phantom in a high-field imaging device. The diffusion phantom created by NIST contains thirteen different tubes. Three neighboring tubes are each filled with one fluid. The remaining tubes are selected and filled pairwise with different fluids. Images are taken at varied levels of magnetization and are used to create a map for the Apparent Diffusion Coefficient (ADC), a measurement that is independent of field strength. These high-field benchmarks can then be used to model low-field brain images. Research can then be done to assess the efficacy of using Artificial Intelligence to generate ADC maps from low-field images.

This ADC value is susceptible to variability from a number of sources. This study seeks to quantify the uncertainty inherent in measuring ADC values. A single tube of a given fluid may exhibit different values depending on its position within the phantom. Within a tube, ADC values are further variable near the tube boundaries, where slight variations in segmentation methods can result in the inadvertent inclusion of image regions outside the desired tube area. Reducing the shape of the image segmentations to exclude problematic boundaries (erosion) can be helpful in ensuring a more robust ADC value, but standards for the appropriate amount of erosion must be established. Using the manual image segmentations as ground truth, ADC values were calculated in different areas of each tube. Measurement uncertainties were quantified using the standard deviation of ADC values computed over the manually segmented areas. In the inner most region of the tube, twice the standard deviation did not exceed 5 mm^2/s. From this, we propose that erosion near the boundaries should continue until two standard deviations of the pixel intensities within a given segmentation does not exceed 5 mm^2/s.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: John Bodenschatz

Academic Institution: University of Cincinnati

Major: Mathematics, Physics

Academic Standing (Sept. 2021): Graduate

Future Plans (School/Career): Pursuing a Ph.D. in Computational Mathematical and Statistical Sciences at Marquette University

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

NIST Research Advisor: Dr. Howard Cohl

Title of Talk: Relations between Carlson’s symmetric elliptic integrals and Legendre’s incomplete elliptic integrals

Abstract:

Chapter 19 of the NIST DLMF (dlmf.nist.gov) provides a detailed summary of the material regarding Legendre elliptic integrals as well as those of different type, symmetric elliptic integrals, which were introduced by Bille Carlson. Symmetric elliptic integrals are free from the modulus and amplitude transformations that complicate Legendre’s theory. Also, for a fixed set of parameters, the symmetric elliptic integrals are symmetric upon an interchange of said parameters. This allows for improved results in computational methods involving elliptic integrals. Elliptic integrals appear in a myriad of applications ranging from the period of the pendulum to elliptic functions (a class of doubly periodic functions that often emerge in fields such as number theory). In Section 19.25(iii) of the DLMF there exists four relations between Carlson’s symmetric elliptic integrals and Legendre’s incomplete elliptic integrals. By interchanging variables within the symmetric elliptic integrals and making use of the properties and transformations of Legendre’s incomplete elliptic integrals, we expand the known set of relations between the two classes of integrals.

This talk will begin with an introduction of the notation, properties, and transformations of Legendre's and Carlson's elliptic integrals. This will be followed by a presentation of the main results, namely the new relations discovered between Carlson's symmetric elliptic integrals and Legendre's incomplete elliptic integrals.

In addition to this project, some work was also done on the relationship between Carlson’s symmetric elliptic integrals and the Weierstrass elliptic functions (in particular, the Weierstrass $\wp$-function). By choosing special lattices for the Weierstrass elliptic function $\wp(z)$, we observe some properties emerge that may further our understanding of the relations presented in Section 19.25(vi) of the DLMF.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Marc Burlina

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

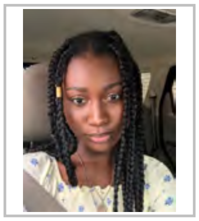
Academic Standing (Sept. 2021):	Sophomore
Future Plans (School/Career):	Finish college, after that not sure.
NIST Laboratory, Division, and Group:	ITL, Software and Systems Division, Information Systems Group
NIST Research Advisor:	Dr. Peter Bajcsy, Dr. Maritoni Litorja
Title of Talk:	Image Fusion Methods for Fluorescence Guided Surgery

Abstract:

Conventionally, during surgery, surgeons must rely solely on their ability to identify anatomical structures of interest (e.g. tumors) under white light illumination. For some operations, such as tumor resection, the accurate identification of these structures is critical to ensuring disease-free patient outcomes. Fluorescence-guided surgery is a medical imaging technique that aids surgeons in identifying structures of interest by marking them with fluorescent dye. Operating rooms are bright, while the light emitted by fluorescent dye can be dim, limiting surgeons' ability to perceive the contrast between fluorescent and surrounding tissue. Additionally, some fluorescent dyes emit light outside the visible spectrum.

Our proposed solution starts with collected co-registered visible light images and images which capture the wavelengths of light emitted by the fluorescent dye simultaneously. The goal is to fuse these images in real time such that the fused image retains the information captured in the visible image while allowing fluorescent tissue to be perceived and interpreted more easily. We approach the blending problem by designing steps for (a) segmenting high intensity fluorescent regions (e.g. tumor regions), (b) finding a color that contrasts highly with surrounding visible tissue, and (c) optimal mapping of fluorescent intensity to color.

Our design uses binary morphology to segment tumors in fluorescent images, the CIELAB color space's ΔE^* color difference metric to find high contrast colors, and alpha blending to integrate the two image modalities. This design yields multiple fusion outcomes dependent on a range of algorithmic parameters. The fusion results will be presented to surgeons who will evaluate their utility and select preferred outcomes. Their feedback will be used to train a deep neural network to fuse images based on preferred outcomes. The results will give insight into the characteristics of image fusion methods that are valuable to surgeons in the operating room.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Khar Aminata Casse

Academic Institution: Montgomery College

Major: Computer Science

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Attend a four-years university to continue Computer Science with a concentration in data Science or Cybersecurity. I am also considering a minor in digital arts.

NIST Laboratory, Division, and Group: Information Technology Laboratory (ITL), National Initiative for Cybersecurity Education (NICE)

NIST Research Advisor: Davina Pruitt and Danielle Santos

Title of Talk: Analyzing the engagement of the K-12 community in cybersecurity: Past efforts and future directions.

Abstract:

The National Initiative for Cybersecurity Education (NICE) is a partnership among government, academia, and the private sector focused on education, training, and workforce development that will strengthen the cybersecurity posture of organizations. This “cybersecurity workforce” includes those whose primary focus is on cybersecurity as well as those in the workforce who need specific cybersecurity-related knowledge and skills to perform their work in a way that enables organizations to properly manage the cybersecurity-related risks to the enterprise. The NICE Strategic Plan outlines the vision, mission, values, goals, and objectives for both the organization and the greater NICE community. The NICE Community Coordinating Council (NICE Community) has been established to provide a mechanism in which public and private sector participants can develop concepts, design strategies, and pursue actions that advance cybersecurity education, training, and workforce development.

The former K12 Working Group, renamed the K12 Community of Interest, is a forum for K12 teachers, school administrators, local and state education agencies, non-profit organizations, federal agencies, institutions of higher education, and others who are interested in sharing and learning how to grow and sustain diverse students pursuing cybersecurity careers through learning experiences, exposure to career opportunities, and teacher professional development. In 2016 a K12 Cybersecurity Education Implementation Plan was developed to establish a coordinated, coherent portfolio of national K-12 cybersecurity education activities so that efforts and assets were deployed effectively and efficiently for greatest potential impact. The intent was to encourage a more deliberate focus among new and existing efforts and create synergies among programs and agencies. This plan was created to implement the NICE Strategic Plan in the K12 ecosystem.

This project will analyze the K12 cybersecurity education landscape in the United States aligned to the National K12 Cybersecurity Education Implementation Plan and review evidence related to the impact of these initiatives, to the extent such information is available. The NICE Program Office and the NICE K12 Community of Interest is eager to learn, “as a nation, what have we done well to build public awareness of cybersecurity knowledge, skills, and careers, and support youth obtaining cybersecurity credentials?”

Research questions guiding this work include:

- Have we and if so, how have we increased cybersecurity career awareness in the U.S.?
- How do youth learn about cybersecurity concepts and cybersecurity careers?
- How is cybersecurity taught in grades K–12?
- What types of instructional materials and curricula have been used?
- What instructional strategies have been used?
- What academic and career pathways have been used?

Using the NICE K12 Cybersecurity Education Implementation Plan as a scaffold, this project sets out to determine what progress has been made over the past five years? What have we done well? What elements and strategies have had the greatest impact? And what elements are strategies should be addressed moving forward?

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Justin Chen

Academic Institution: University of Virginia

Major: Computer Science

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Attend graduate school to study Computer Science

NIST Laboratory, Division, and Group: Information Technology Lab, Computer Security (773), Security Testing Validation and Measurement

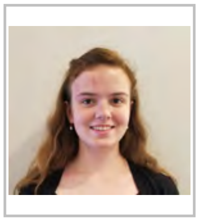
NIST Research Advisor: Chris Celi

Title of Talk: Client Development for the Entropy Source Validation Server

Abstract:

With the incoming age of quantum computing and cryptocurrencies, computer security is becoming more important than ever before. One crucial aspect of computer security is entropy and the ability to generate truly random inputs, like cryptographic keys and initialization vectors. Deterministic Random Bit Generators (DRBGs) make use of properties in popular algorithms (AES and SHA) to turn an entropic seed into many more random values that can be used for inputs. In the generation of these seeds, it is important that they are created by an entropy source that is capable of producing high-entropy (unpredictable) bits.

The ESV (Entropy Source Validation) server is part of a recently established protocol and currently performs tests and validations of modules containing these entropy sources sent in by companies and third-party labs. However, current validations methods are not automated, so users will benefit from improvements to the process.. Therefore, to better streamline the process for entropy validations and integration testing, a client must be developed that is fast, secure, and functional. For security, the client implements a two-factor authentication method that includes mutual TLS and an 8-digit TOTP algorithm that is based on RFC 6238. Furthermore, the user must have minimal interaction with the client while still being able to perform various operations according to their needs, including certification, file uploads, and status checks. Finally, API requests to the server are multi-threaded to handle uploads of large amounts of test data in a short amount of time and configured to be sent to the server's IPv4 address.



SURF Student Colloquium

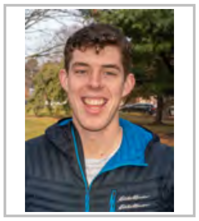
NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Elizabeth Euwart		
Academic Institution:	Worcester Polytechnic Institute	**Major:**	Mathematical Sciences
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Graduate School for Mathematics		
NIST Laboratory, Division, and Group:	ITL, Applied & Computational Mathematics		
NIST Research Advisor:	Prof. Michael Mascagni		
Title of Talk:	Probability Distribution of Number of Steps in Walk on Spheres Method		

Abstract:

Walk-on-spheres is an algorithm used to approximate solutions to boundary value problems for partial differential equations. Walk-on-spheres is a Monte-Carlo method in which a sequence of spheres is generated, each sphere centered at a random point on the surface of the preceding sphere, until the spheres reach a location within some error bound of the boundary. This process is repeated many times and the first passage points of the Brownian motion are used to approximate the solution. Walk-on-spheres is used in the NIST ZENO code to calculate material properties.

To investigate the distribution for the number of steps (N) in the walk-on-spheres, we used a simplified model, the half-space, in which the boundary is the x-y plane. In this simplified model, the ratio of the radius of a sphere generated in one step to the radius of a sphere generated in the previous step follows a uniform distribution. Iterated integration over this ratio was used to determine the probability density function for N. A simulation in R of the walk-on-spheres for the half-space model was used to test this result. This distribution allows us to accurately calculate the probability of a certain number of steps in walk-on-spheres in the simplified model and improves our understanding of the behavior of the walk-on-spheres algorithm.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Jason Eveleth			
Academic Institution:	Brown University	**Major:**	Math-Computer Science
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Pursue a PhD in math or computer science		
NIST Laboratory, Division, and Group:	Information Technology Lab, Applied and Computational Mathematics Division, Mathematical Analysis and Modeling Group		
NIST Research Advisor:	Dr. Anthony Kearsley		
Title of Talk:	Grain coarsening in voronoi diagrams		

Abstract:

Imagine a city map that colored each house differently based on the nearest post office. That map would partition the city into colored regions, which approximate a Voronoi diagram, a concept that often appears in science and engineering. These diagrams appear in the network of crystals in heated metal, the bubbles in soap foams, and disease outbreaks originating from different sources.

Motivated by Voronoi diagrams in the study of soap foams, we investigate the evolution of these diagrams over time. These diagrams often evolve by minimizing the total length of the boundaries of the regions (referred to as the perimeter). However, the problem becomes further complicated by requiring that none of the regions shrink and disappear, which often happens when this type of evolution is unconstrained. We can generalize the post office locations as a collection of coordinates (referred to as sites). We are interested in an objective function whose input is the sites and whose value is the length of the perimeter of the diagram summed with an optional repulsion term, which keeps the sites from getting too close. This function is differentiable, so we can use many gradient descent methods to carry out the evolution. Interestingly, these different methods have different behavior. For example, using constant step-size gradient descent gives different behavior than using the Barzilai-Borwein method.

The objective function is highly nonlinear and nonconvex, so different methods and initial conditions yield different solutions. For each of these methods, we collect geometrical and topological statistics about the boundary network over time. Our goal is to understand how these diagrams change over time. Overall, it is important to understand the evolution of Voronoi diagrams because of the implications in metallurgy and the study of soap foams.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Nishaant Goswamy

Academic Institution: New Jersey Institute of Technology **Major:** Cybersecurity and Privacy

Academic Standing (Sept. 2021): Graduate Student

Future Plans (School/Career): Attending graduate school to pursue a Master's Degree in Cybersecurity and Privacy.

NIST Laboratory, Division, and Group: Information Technology Laboratory, Advanced Network Technologies Division, Emerging Network Technologies Group

NIST Research Advisor: Lotfi Benmohamed, Davide Pesavento, and Junxiao Shi

Title of Talk: Named Data Networking (NDN) Dissector for Wireshark

Abstract:

In the current Internet architecture, TCP/IP allows for point-to-point communication between entities. However, the Internet has moved forward to a more advanced state with mobile devices, video streaming services, IoT (Internet of Things) devices, and connected cars. Therefore, the research on Name Data Networking (NDN) focuses on designing a new network architecture that names the chunks of data in the conversation with additional metadata. For example, instead of embedding the details of the content in the higher-layer protocols, the NDN packet is directly addressed as “/videos/WidgetA.mpg/1/3”, which would indicate that this is segment 3 of version 1 of the video. The NDN architecture focuses on forwarding data based on its name rather than which specific route to take. Also, since every data packet has a unique name, the data packet can be cached within the network for future requests. NDN packets feature enhanced security by requiring the producer to cryptographically sign all data packets sent, so that their authenticity can be verified by the consumers.

My research project focuses on developing a new NDN dissector for Wireshark to analyze network traffic between entities communicating using the latest version of the NDN protocol. Wireshark is a popular open-source packet analyzer software that can analyze packet data using dissectors. Using Lua, a lightweight scripting language, I wrote a dissector that can parse and organize the captured network traffic into a readable format. The parser can read NDN packets over Ethernet, UDP, and TCP by displaying the name components and additional metadata such as the signature information of the packet. The parser can also reassemble fragments of the NDN Link Protocol, which fragments large network layer packets to fit under the Maximum Transmission Unit (MTU) size limit. In the future, this dissector can be very effective in examining and troubleshooting network traffic when more devices start communicating using the NDN protocol.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Muktaka Bhushit Joshipura

Academic Institution: Georgia Institute of Technology

Major: Computer Science

Academic Standing (Sept. 2021): 4th year

Future Plans (School/Career): Graduate study in a PhD program

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

NIST Research Advisor: Dr. Timothy Blattner

Title of Talk: Streaming Linear Algebra

Abstract:

Hedgehog is a parallel computing library that allows programmers to write high-level data-flow graph representations of algorithms while allowing them to achieve a high degree of compute resource utilization with easy extension to heterogeneous computers. Hedgehog-MatrixLib, a linear algebra library built on top of Hedgehog, extends the benefits of Hedgehog to linear algebra operations by streaming the results, emitting blocks of the result as soon as they are computed. Hedgehog-MatrixLib's performance has been positively compared to the OpenBLAS library on the linear algebra algorithms of GEneral Matrix-Matrix multiplication (GEMM) and GEneral TRiangular Factorization (GETRF, LU decomposition with partial pivoting).

The Hedgehog-MatrixLib represents its linear algebra routines as dataflow graphs. The output of one dataflow graph can be used to feed into the input of another. In this study, we explore the benefits of using this data streaming approach to perform linear algebra operations in succession to try and maximize the overlap time of the execution of the operations to minimize the end-to-end compute time. To this end, we examine methods of maximizing parallelism at the interface of GEMM and GETRF, and GEMM and GEneral Matrix-Vector multiplication (GEMV). Several factors impact the overall performance of these data flow graphs, such as block size, traversal patterns, thread configurations, and decomposition strategies between operations. As a result of this work, we present performance metrics comparing the end-to-end execution times of the same algorithms using OpenBLAS. Additionally, we measure the effective overlap of computation between successive linear algebra operations.

This study shows how the data-flow graph representations of algorithms can be leveraged to increase parallelism on linear algebra routines. In particular, how the use of data flow can be used to target the critical path between operations. Further efforts can be made to realize these benefits to a greater degree with heterogeneous platforms.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Ray Karyshyn

Academic Institution:	University of Maryland, Baltimore County	**Major:**	Computer Science
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Finish undergraduate studies and pursue a career in computer science and cybersecurity.		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Software and Systems Division, Information Systems Group		
NIST Research Advisor:	Alden Dima		
Title of Talk:	Comparative Evaluation of XML and JSONL for Technical Data		

Abstract:

Technical data is often provided in Comma-Separated Values format; however, using a self-describing structure, such as the eXtensible Markup Language (XML) or JavaScript Object Notation (JSON), simplifies the processing and transformation into other formats. For past work in the Material Genome Initiative, the National Institute of Standards and Technology has decided to take an XML-based approach—evident in the case of the Configurable Data Curation System. A newer approach to utilizing JSON is newline-delimited JSON (aka JSON Lines or JSONL), where each line is a valid JSON value. The purpose of this study is to perform a comparative evaluation of current XML and JSONL approaches by investigating clarity, usability, performance, and scalability.

Both qualitative and quantitative methods were used to examine the completion of five tasks, which explore typical aspects and operations of self-describing structures: schemas, file generation, insertions and selections with database systems, and transformation into other formats. Common qualitative themes that arose when working with JSONL approaches were adequate documentation and readable code, whereas XML approaches usually involved the use of more online resources and extra steps. In the quantitative measurements, it was observed that XML approaches took longer to execute and required a higher memory usage than the JSONL approaches. The results show that JSONL approaches frequently surpass XML ones in the categories of clarity, usability, performance, and scalability. The results of this study will serve to guide future system development.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Sophie Koh			
Academic Institution:	Amherst College	**Major:** Physics and Computer Science	
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	ITL, Applied and Computational Mathematics Division, High Performance Computing and Visualization Group		
NIST Research Advisor:	Justyna Zwolak		
Title of Talk:	Improving Machine Learning Heuristic Metrics for Solitonic Excitation Classification in Bose-Einstein Condensates		

Abstract:

Bose-Einstein condensates (BECs) are ultracold collections of atoms which exhibit macroscopic quantum effects. As such, BECs are an ideal environment for creating quantum solitons—robust, localized waves which retain their size and shape as they travel. Dark solitons are associated with a local decrease in condensate density, visible in images of a BEC. With a dataset of labeled images from BEC experiments, we trained a machine learning (ML) model to locate solitons. Though multiple solitonic excitations such as kink solitons, solitonic vortices, and soliton rings represent distinct physical states, the ML system identified them all as solitons due to their similar visual features. Given the location of a potential solitonic excitation, we created a heuristic metric to measure confidence in presence of a soliton. The metric sums the images vertically and uses a five-parameter fit to a 1-D function describing an idealized soliton profile. While the proposed metric is very effective with kink solitons which remain vertically consistent, it has limited applicability to distributions that vary vertically, as seen with solitonic vortices. With the goal to determine the specific type of solitonic excitation, we fit the metric to separate segments of each image. If the metric parameters varied among the image segments, we analyzed the differences between those parameters to distinguish solitonic vortices from kink solitons. Through using machine learning models to locate positions of solitonic excitations and improving the heuristic metric to distinguish between types of solitonic excitations, the integration of machine learning and physics-based heuristics improved our classification and detection of solitonic excitations in BEC images.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: John Kucera

Academic Institution: University of Maryland Global Campus **Major:** Computer Science

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Graduate in 2022 with Bachelor of Science degree, then find a full-time job in Computer Science field.

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

NIST Research Advisor: Derek Juba

Title of Talk: Investigation of Floating-Point Reproducibility

Abstract:

Scientific computations make heavy use of floating-point arithmetic, which approximates real number arithmetic. Being an estimate, floating-point arithmetic generally incurs errors. These errors can differ between systems. Tools have been developed to quantify the uncertainty caused by the errors. One such tool is CADNA (Control of Accuracy and Debugging for Numerical Applications) which performs calculations several times with random rounding to provide a distribution of results. This can be used to compute a standard deviation for the floating-point approximation error. For this project, I used the CADNA tool to analyze a program which simulates a biological neural network. The simulator uses floating-point arithmetic to solve a sequence of differential equations.

The output of this particular program is significantly changed when running it with different CPUs. By running the neural simulator with CADNA, I was able to produce a mean and standard deviation for the floating-point output. For each CPU, I graphed the mean along with an uncertainty bound of plus or minus the standard deviation. I also altered other parameters in the simulator to observe their effect on the output. I found that the values of the altered simulation fell outside of the original standard deviation envelope.

When researchers try to reproduce a computational experiment and fail to exactly replicate the original results, it is uncertain whether it is due to human error or differences between systems. By using a tool like CADNA, researchers can check whether their results lie within the expected variation between different systems. Based on this, they can conclude whether they successfully reproduced the experiment.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Peter Lef		
Academic Institution:	Clarkson University	**Major:**	Mathematics
Academic Standing (Sept. 2021):	Freshman		
Future Plans (School/Career):	Unknown; maybe research in industry in some math- and CS-related field		
NIST Laboratory, Division, and Group:	Information Technology Laboratory, Applied and Computational Mathematics Division, Mathematical Software Group		
NIST Research Advisor:	Gunay Dogan		
Title of Talk:	Denoising and Inpainting Material Microstructure Orientation Maps using Differential Equations		

Abstract:

In material science, a "crystal" is a solid material with a highly regular and repetitive molecular arrangement. Many industrially-used materials are polycrystalline, composed of multiple crystals ("grains") with varying spatial orientations. A material's macroscopic properties depends on its grain orientations, and material science often involves analysis of "orientation maps" depicting the grain orientation at every point in a material sample. Methods of obtaining these orientation maps are imperfect; the resulting maps may contain some inaccurate data ("noise"), and data may be missing at some points.

The problems of correcting anomalous data ("denoising") and filling in missing data points ("inpainting") in orientation maps has similarities to those in natural images, and methods from computer vision fields exist with limitations. Simpler local averaging techniques for denoising often blur sharp edges, damaging critical features such as grain boundaries. More complex, edge-preserving techniques rely strongly on input parameters for which finding optimal values is an open problem. We propose a partial-differential-equation (PDE) based denoising method which preserves edges without strong reliance on parameter selection, and which can be used for limited inpainting. This is achieved using an iterative PDE-based algorithm for minimizing total variation (effectively reducing image gradients by diffusing the image pixels), modified with a weight factor to reduce its effect on grain boundaries.

We implemented this algorithm in Python for traditional (2-spatial-dimension) and volumetric (3-spatial-dimension) images. Experiments are in progress; initial experiments on 2D images were performed by adding noise to and removing data points from artificially-produced, clean, ground truth orientation maps, and comparing denoised and inpainted results with the original ground truth maps. In most cases, we found that our method produced results closer to the ground truth than other methods. Inpainting was found appropriate for maps with many scattered missing data points, but did not perform as well for large contiguous missing chunks.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Denis Liu

Academic Institution: Arizona State University **Major:** Computer Science

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Pursue Graduate School

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

NIST Research Advisor: Min Ding

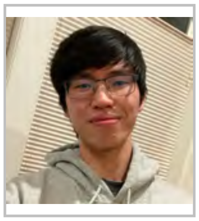
Title of Talk: cuML Benchmark Evaluation on Nisaba GPU Platform

Abstract:

Graphics Processing Units (GPUs) can be used in the place of Central Processing Units (CPUs) to accelerate data analytics and machine learning. RAPIDS is a suite of software libraries from NVIDIA for accelerating data science and analytics on GPUs. A library from RAPIDS, cuML, implements machine learning algorithms and mathematical primitive functions in a manner similar to the scikit-learn library. It allows users to run traditional tabular machine learning tasks on GPUs without needing to delve into the details of low-level CUDA programming. The purpose of this investigation is to develop benchmark machine learning algorithm testing on NIST's Nisaba GPU cluster and compare performance of cuML and scikit-learn.

Both generated data and real data are used to benchmark clustering, dimensionality reduction, and regression/classification machine learning algorithms. Algorithms are benchmarked by measuring the time the algorithm takes to fit the data. Each fitting is repeated thirty times and averaged to ensure accuracy. The results obtained indicate speedup of cuML compared to scikit-learn; for example, cuML KMeans clustering and linear regression performed around 200 times faster when dataset size and dimensionality were high. Additionally, the results show that speedup of cuML increases as dataset size and dimensionality increases. On the other hand, when dataset size and dimensionality are small, scikit-learn can be faster.

Further, cuML supports multi-GPU and multi-node operations in conjunction with Dask (Dask cuML). For its supported algorithms, Dask cuML will be benchmarked alongside cuML and scikit-learn. Ultimately, this benchmarking evaluation can be used to determine when it may be fit to use cuML, Dask cuML, and scikit-learn.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Elvin Liu

Academic Institution: University of Maryland, College Park

Major: Computer Science, Math

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Entering industry to work in computational modeling then possibly attending grad school

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

NIST Research Advisor: Joe Chalfoun, Adele Peskin

Title of Talk: Evaluation of the FogBank cell segmentation method ported to Python

Abstract:

Automated cell segmentation is a vital aspect for the analysis of individual cells within a cell sheet. FogBank is an existing method that produces highly accurate cell segmentations from confluent cell sheets, and can be used on images of multiple cell lines and a variety of image modalities. However, the existing code base is written entirely in MATLAB, which is unsatisfactory for those working within the Python software pipeline or people who prefer open-source software. The goal of this project is to produce a Python port of the FogBank method that matches the existing MATLAB code to high accuracy, while also ensuring that the resulting code is performant in regards to both speed and memory usage.

In order to do this, we use a certain number of test images of various cell sheets along with randomized parameters and compare the results of the MATLAB and Python implementations. In particular, two aspects of the FogBank code are being evaluated: the Empirical Gradient Threshold foreground-background separation, and the actual FogBank segmentation. This comparison is done by computing the Adjusted Rand Index, which measures similarities between segmented images. Ultimately, we aim to produce a Python port that segments images to at least 99% similarity to the existing MATLAB code. Additionally, we evaluate the performance of the Python port in terms of both its speed and memory usage, to ensure that it is not significantly worse than the MATLAB code in either of these regards. The final port will be useful to researchers interested in using FogBank in Python pipelines or who desire non-proprietary software.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Matteo Marchi

Academic Institution: University of Maryland **Major:** Computer Engineering

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Masters / Doctorate in Computer Engineering

NIST Laboratory, Division, and Group: Information Technology Laboratory, Management Resources - 135 Information Services Office (Museum & Library), Office of Information Systems Management - 183 - Application Systems

NIST Research Advisor: Paula Deutsch

Title of Talk: Web Archiving NIST's iNet with Brozzler

Abstract:

In our current information age, a veritable torrent of web content is created and destroyed as web pages are constantly in flux with updates and replacements. Web content is highly vulnerable to deletion and loss, which is why web archiving is so crucial. The NIST Research Library and Museum is attempting to resolve this problem specifically to preserve web content on NIST ’ s internal site (iNet) in a secure and cybersafe fashion.

Web archiving involves the capture and preservation of digital data, making it accessible for the long term by saving the content in a standard format which will reproduce the information in the future, enduring changes in technology. To preserve iNet information, our group has used Brozzler, a distributed web crawler that uses a browser to fetch web content for internal archiving. Using web archiving tools like Brozzler, we can prevent the loss of essential documents, announcements, and research on iNet, creating an autonomous process that can archive pages and store them for generations to come.

Unlike proprietary alternatives, Brozzler offers private web archiving of internal sites, but comes at several disadvantages. Firstly, Brozzler was designed to archive public sites, and only offers limited support for archiving sites that require authentication. Brozzler can provide the SAML credentials required for access to iNet, but randomly loses access. Similarly, this issue occurs when attempting to archive videos, as SAML authentication is not built into the integrated code Brozzler uses to connect to YouTubeDL, a video-archiving utility. Lastly, Brozzler ’ s integrated dashboard for viewing stored pages is unstable, often failing to replay stored “ crawls. ”

If NIST continues with Brozzler, it will be crucial to redesign the dashboard into an internal tool for stable viewing and storage of pages, and edit the Brozzler code to better work with iNet ’ s more secure SAML authentication.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Lindsay Marean		
Academic Institution:	University of Oregon	**Major:**	Computer and Information Science
Academic Standing (Sept. 2021):	Graduate		
Future Plans (School/Career):	Software Developer		
NIST Laboratory, Division, and Group:	ITL, IAD, Retrieval Group		
NIST Research Advisor:	Ian Soboroff		
Title of Talk:	Inter-Annotator Agreement for Recognizing Ultra Fine-grained Entities		

Abstract:

Knowledge base population (KBP) is an area of research within natural language processing that involves recognizing entities and entering information about them in a knowledge base. Entity detection, coreference, and entity type tagging based on a detailed ontology are subtasks in KBP, and they are targeted by NIST's Recognizing Ultra Fine-grained Entities (RUFES) task, now in its second year. RUFES uses "gold" human-annotated datasets for participants to use in training their systems and for scoring participants' submissions on a test dataset; the quality of the gold dataset sets an upper bound on how well systems can be expected to perform. A high level of inter-annotator agreement (IAA) demonstrates replicability of human annotations based on the ontology and annotation guidelines. IAA measures of different aspects of the annotation task can be used to determine components of the guidelines and ontology that can be refined.

The RUFES 2020 gold dataset was first annotated by annotators with no training in linguistics, then revised in a second pass by the computational linguist who authored the guidelines and fine-grained ontology. The first-pass and second-pass annotations are compared in order to find precision, recall, and F1 scores. IAA measures are taken for hit/misses in mention detection, type classification, and coreference.

Differences between first-pass annotators and the second-pass annotator for the RUFES 2020 dataset indicate inconsistencies in choosing which entities are taggable. A qualitative analysis of the annotation guidelines and comparison with other KBP guidelines indicates that referentiality is a complex concept for annotators.

Findings from RUFES 2020 IAA measures will be used to guide revisions to subsequent RUFES task implementations, and this study establishes protocols that can be used in this and future years to measure IAA and use the results to refine the ontology, the annotation guidelines, and annotator training.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Connor Mooney

Academic Institution: George Mason University

Major: Mathematics

Academic Standing (Sept. 2021): Senior

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

NIST Laboratory, Division, and Group: ITL 771.03

NIST Research Advisor: Lucas Brady

Title of Talk: Lefshetz Thimble Quantum Monte Carlo for Spin Systems

Abstract:

Quantum Monte Carlo methods are effective tools for simulating various quantum phenomena stochastically with classical computers. However, these methods fall short for classes of quantum systems with what is called a sign problem, in which the sampling distribution one wishes to replicate is not positive definite. Solving the sign problem generically is known to be NP-hard. However, various techniques can be used to mitigate it under some conditions. One such technique is called Lefshetz Thimble Monte Carlo and has been used extensively in high energy and condensed matter physics.

In this project we investigate how to adapt this technique for use in analyzing spin systems. Various difficulties arise in the process of doing so, due to the fact that the technique requires a continuous state space, while those of spin systems are discrete. As such, some changes were necessary to make this method work with spin systems. We apply this adapted technique to a simple d-level spin, and evaluate its prospects in ameliorating the sign problem for more complicated setups.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Erchis Patwardhan

Academic Institution: UC Berkeley **Major:** Computer Science

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Industry

NIST Laboratory, Division, and Group: Information Technology Labratory

NIST Research Advisor: Dr. Spencer Breiner

Title of Talk: Implementing Parameterised Map Construction for use in Backpropogation Algorithm

Abstract:

A recent paper written by Geoff Cruttwell et. al has demonstrated the use of category theory in neural networks. Specifically, how the backpropagation/training algorithm can be thought of as a "parameterized map construction". The "Parameterized Map Construction" is useful to properly abstract the many parameters needed for the backpropagation/training algorithm to work, which is how the neural network learns to classify data. Our work focused on building upon the Category Theoretic machinery proposed in Cruttwell's paper and we wanted to implement it in an AlgebraicJulia framework. My talk will summarize the main points from Cruttwell's paper and discuss the details surrounding our partial implementation.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Karol Sadek

Academic Institution: University of Maryland, College Park **Major:** Statistics and Economics

Academic Standing (Sept. 2021):

Future Plans (School/Career): Graduate School (currently unsure of which path)

NIST Laboratory, Division, and Group: Information Technology Laboratory, Statistical Engineering Division - 776, Statistical Design, Analysis, and Modeling Group - 04

NIST Research Advisor: Dr. Adam Pintar

Title of Talk: Designing Experiments to Estimate the Non-linear Response of a Spectroradiometer

Abstract:

Spectroradiometers, such as found on the Orbiting Carbon Observator-2 (OCO2), can be used to measure averaged carbon dioxide (CO2) mass fractions in columns of the atmosphere. Before these instruments leave the Earth's surface, they must be calibrated, and an important part of that calibration is quantifying the non-linearity of the instrument's response to light.

This work builds on an ongoing collaboration between ITL and PML to leverage maximum likelihood and the statistical bootstrap in the problem of estimating the non-linear response of an instrument as well as quantifying the uncertainty in that estimate. The envisioned calibration experiments involve an integrating sphere in which the light level presented to an instrument is varied by turning nominally identical lamps on or off (or opening or closing shutters). This work is aimed at optimally designing these experiments, i.e., maximizing information content for a fixed number of experimental runs. The work proceeds in two phases.

In the first phase we consider how to measure the information content of an experiment. A common approach is to consider a summary of the covariance matrix for the estimated parameters of the calibration model (such as the determinant or the trace). The bootstrap has worked well in some situations to estimate this matrix but is computationally burdensome. We have found that the inverse second derivative matrix of the log-likelihood, evaluated at the maximum likelihood estimate may be used for design purposes, but not uncertainty quantification more generally.

In the second phase we consider the task of searching for an optimal design using genetic algorithms. Starting from an initial design, rows of the design matrix are replaced at random from a candidate list, which produces a first generation of designs. The best designs in the first generation are retained, and the process repeats.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name: Peter Shin

Academic Institution: George Mason University

Major: Applied Computer Science

Academic Standing (Sept. 2021): Senior+

Future Plans (School/Career): Apply for the accelerated master's program

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

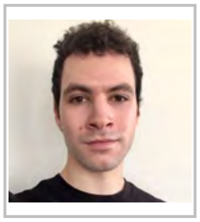
NIST Research Advisor: John Penczek

Title of Talk: Evaluating Augmented/Virtual Reality Visual Performance

Abstract:

With the emergence of Augmented and Virtual Reality (AR/VR) technologies, companies are incorporating the use of mixed reality in different fields such as military, medicine, and education. One of the big technical challenges for AR/VR devices is to avoid a form of cyber sickness caused by a phenomenon known as the vergence-accommodation conflict (VAC). To perceive depth in a real 3D environment, the eyes have to constantly adjust. These adjustments involve both converging the eyes towards the object (vergence) and bending the lens to focus (accommodation). In the virtual world, AR/VR devices typically have a fixed focus distance. But the 3D image content adjusts the vergence angle to simulate depth, which is often mismatched with what the human vision system would expect in the real world. The brain is especially sensitive to this mismatch between vergence and accommodation when working at close distances for long periods, such as in surgery.

This project involves developing a measurement system to evaluate the visual performance of AR/VR devices by generating 3D stereo pair images onto a head-mounted display. These images can be manipulated by adjusting the binocular disparity, or the offset between two images, to simulate depth. The disparities can then be measured by a robot-based optical test system. A commercial Augmented Reality device was used for this project, which incorporated sensor fusion technology to facilitate human-machine interaction. There are a variety of methods to communicate with the device and interface with its sensory information. We pursued an open-source approach using programs such as Unity and the Universal Windows Platform in Visual Studio. Controlling the image content to the device at a low-level is the first step in the development of this project.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Ramon Suris-Rodriguez		
Academic Institution:	Towson University	**Major:**	Mathematics
Academic Standing (Sept. 2021):	Graduate		
Future Plans (School/Career):	Employment at the Johns Hopkins University Applied Physics Laboratory and enrollment into a graduate program in Applied Mathematics		
NIST Laboratory, Division, and Group:	ITL, Applied and Computational Mathematics Divison, Mathematical Software Group		
NIST Research Advisor:	Dr. Howard Cohl		
Title of Talk:	Integral and q-Integral Representations of the Askey-Wilson Polynomials		

Abstract:

The Askey-Wilson polynomials are a family of orthogonal polynomials that typically are represented as a terminating basic hypergeometric series. Basic hypergeometric series, and by extension the Askey-Wilson polynomials, appear in the mathematics of q-calculus, a difference calculus that generalizes the more widely known differential and integral calculus taught in high school and university. For example, the q-derivative is a difference quotient dependent on the parameter q. However, in the limit as q goes to 1, the q-derivative converges to the well-known differential derivative operator. In the literature, it is well-known that basic hypergeometric series can be transformed into integrals, q-integrals, and other basic hypergeometric series. Therefore, the Askey-Wilson polynomials can be represented as an integral, q-integral, and other terminating and nonterminating basic hypergeometric series. What is unknown is an exhaustive list of all possible representations for each aforementioned type of representation of the Askey-Wilson polynomials.

In this talk, we will go over the basics of q-calculus, basic hypergeometric series, and the known representations of the Askey-Wilson polynomials. We will then pivot to the results of our work to exhaustively discover and list the integral and q-integral representations for the Askey-Wilson polynomials.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Selena Xiao

Academic Institution: University of Maryland, College Park

Major: Computer Science

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): I plan on pursuing a career in computer science and cybersecurity

NIST Laboratory, Division, and Group: Information Technology Laboratory, Computer Security Division, Security Engineering & Risk Management Group

NIST Research Advisor: Hung Trinh, Kate Schroeder

Title of Talk: Using Natural Language Processing to Supplement a Cyber Incident Graph Database

Abstract:

There is a growing need for relevant information in Cybersecurity Risk Analytics to combat and prevent cyber incidents. To address this need, previous work focuses on developing a graph database that pulls together data from multiple cyber incident data repositories and analyzes trends between structured data fields. The data is visualized in Neo4j as nodes and relationships and can be queried to find patterns between the nodes. Natural Language Processing was previously used to match similar incidents reported in different datasets to clean up duplicate data entries.

Currently, our team is supplementing the previous work by using Natural Language Processing to extract data from the unstructured text fields. We are using IBM Watson Knowledge Studio to train and automatically detect relevant keywords within the unstructured text, for example, the names of Advanced Persistent Threats, their methodologies, and the mitigations used. Training involves creating keyword categories (APT, Methodology, Mitigation), dictionaries containing a list of real-world terms within each category, and unstructured text documents. The documents are then manually annotated in Watson Knowledge Studio, highlighting keywords and relationships between keywords. The data is extracted through Watson Discovery with Natural Language Understanding. This process continues with Neo4j to obtain additional information from the data sources that were not already predefined and provide additional detail for graph visualization and queries. The product of this project adds more layers of information through the combined use of Natural Language Processing and graph visualization to address cyber risk.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Joshua Zarb

Academic Institution: University of Maryland, College Park

Major: Computer Science

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Become a Software Enginner after receiving my Bachelor Degree

NIST Laboratory, Division, and Group: Information Technology Laboratory

NIST Research Advisor: Dr. Ian Soboroff

Title of Talk: Indicating relevance in search engine evaluation

Abstract:

In this project we wanted to measure search engine accuracy. To do this we need to ask people to indicate whether various documents are relevant or not to a given query. This idea is dependent on what information the user wants from the documents. We explored two ways in which the user could do this. The first would be to review a document and click a button to show that the document was relevant and the second would be to highlight important words that make the document relevant. Highlighting takes longer than clicking, and so the user will not be able to review as many documents for relevance. On the other hand, highlighting tells the researcher more about what made the document relevant to the user. The question then becomes does the benefit from highlighting overcome the cost?

To answer this question we first created a programming project in React where the user is able to highlight key terms in a text. We then designed an experiment where users were shown different documents and we asked them randomly to highlight the document or click the button when the document was relevant. We will measure how much longer highlighting takes, and hypothesize that it is longer but less than twice as long.

Material Measurement Laboratory (MML) Participants

Ilyas Adnane

Katherine Boyd

Alexandria Brady-Mine

Ethan Chen

Daniel Coile

Maurice Curran

Daniel Delgado

Katherine Dura

Jalen Garner

Wyatt Gibbs

Catherine Gill

Devin Golla

Eleanor Grosvenor

Ross Gunther

Bliss Han

Noah Hobson

Jordan Hoffman

Material Measurement Laboratory (MML) Participants (continued)

Jesse Ji

Jennifer Li

Richard Ma

Daniel Markiewitz

Miyu Mudalamane

Sareet Nayak

Anika Rajamani

Malaak Saadah

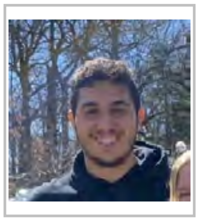
Logan Saar

Priya Shah

Michaela Staab

Chloe Taylor

Alex Wang



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Ilyas Adnane

Academic Institution: University of Michigan - Ann Arbor **Major:** Physics

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate school to pursue a Ph. D

NIST Laboratory, Division, and Group: Material Measurement Laboratory; Chemical Sciences Division; Chemical Informatics Group

NIST Research Advisor: Jacob Monroe

Title of Talk: Calculating Entropies and Identifying Key Elements of Liquid Structure with Normalizing Flows

Abstract:

Solvating a solute in a solvent is a crucial process in many different disciplines. For example, pharmaceutical companies utilize this information to understand how medications distribute throughout the human body, oil companies to refine crude oil into petroleum, and environmentalists for creating treatments for the decontamination of water. During the process of dissolving a solute in a solvent, the interactions are affected by the solutes interacting with each other, as well as the solvent as a whole. “Solvent-mediated” interactions, as they are known, can become increasingly complex and difficult to accurately model due to the large number of degrees of freedom involved. Typically, though, we can identify a few key variables that capture the key physics of the solvation process, but they are not easy to discover. Using Monte-Carlo techniques to simulate molecular configuration, we can then utilize normalizing flows, a recent development in machine learning, to discover the key interactions during this process. The interactions will then allow us to surmise the entropy changes of the system, a crucial component for calculating the free energy changes associated with the solvation process. Solving for the free energy differences will then allow us to extract the thermodynamic properties governing any solvation, providing useful information to many different fields. To begin, we find the some of the best practices for applying normalizing flows to bulk fluids for the purpose of calculating entropy. By varying coordinate representations of a given system, we are able to compare and contrast the accuracy of each representation. Theoretically, the result should be unaffected by the coordinate representation, but we find that the entropy change calculated does vary as a result of the different representations.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name: Kate Boyd

Academic Institution: Colorado State University

Major: Chemical and Biological Engineering

Academic Standing (Sept. 2021): Senior

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

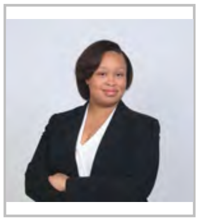
NIST Laboratory, Division, and Group: Materials Measurement Laboratory, Applied Chemicals and Materials Division, Thermodynamics Research Center

NIST Research Advisor: Demian Riccardi

Title of Talk: Estimating HDX-MS of ERK2 from multi-microsecond molecular dynamics simulations

Abstract:

Extracellular signal-regulated kinase 2 (ERK2) is a protein kinase being looked at as a target for inhibitor development in cancer treatment. Many protein kinases have large conformational differences between active (phosphorylated) and inactive (unphosphorylated) states. The structural similarity of active and inactive ERK2 has led to the hypothesis that dynamics play a role in enzymatic activity. Molecular dynamics simulations were run for three states of ERK2 modeled from two crystal structures (protein database ids 2erk and 5umo): the dually phosphorylated (2erk_2p) and unphosphorylated (5umo_0p) states provide endpoints of the phosphorylation process; the third state (2erk_0p) models the unphosphorylated state starting from the 2erk_2p state with the phosphate groups removed. The three conformations were simulated for around 10 microseconds each at four different temperatures ranging from 285-330K to compare with experimental data from hydrogen deuterium exchange mass spectrometry (HDX-MS). The trajectories were analyzed to distinguish "open" (exchangeable) and "closed" (unexchangeable) states and determine the frequencies of each amide in either state. From these analyses we can better understand the role of ERK2 dynamics in enzymatic activation.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Alexandria Brady-Miné

Academic Institution: University of South Florida

Major: Mechanical Engineering

Academic Standing (Sept. 2021): Junior

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

NIST Laboratory, Division, and Group: Materials Measurement Laboratory

NIST Research Advisor: Dr. Harold Wickes Hatch

Title of Talk: Uncertainty Quantification in Transition-Matrix Monte Carlo Simulations

Abstract:

Monte Carlo simulations are widely used in computer simulations of liquids and soft matter, phase equilibrium, and self assembly. These simulations require a random number generator to simulate a desired probability distribution. Due to the nature of the random number simulation, each random seed has a different result. Error calculations are key in determining if simulations with the same parameters give statistically identical results.

Monte Carlo simulations of molecules are made up of small perturbations to the system and produce correlated data. In this project, we utilized two methods to determine the error of the mean. The simplest approach is to run multiple simulations with different random seeds and perform statistics on the independent averages of those simulations. Alternatively, the blocking method was used to calculate the uncertainty of the mean using one simulation. The correlated simulation data were grouped into block averages that become uncorrelated when the blocks are sufficiently sized. While the blocking method is more efficient because it only requires one simulation, the block size must be chosen carefully and the blocking method needs to be validated for use in flat histogram methods that compute free energies.

We compare and contrast these two uncertainty methods in a model Lennard-Jones fluid system with liquid and vapor coexistence using both canonical and grand canonical ensemble simulations to better understand the current methods to calculate uncertainty and to develop a method to calculate uncertainties in flat histogram transition matrix monte carlo with one simulation using the blocking method.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Ethan Chen

Academic Institution: Purdue University

Major: Biochemistry

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate School

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

NIST Research Advisor: Frederick Phelan Jr. and Lilian Johnson

Title of Talk: Modeling Polycarbonate Confined Between Crystalline Silica Surfaces

Abstract:

Polymer composites are a class of multiphase materials in which a polymer matrix is reinforced with either a fiber or filler phase. They are known for their high strength to weight ratio, stiffness, and corrosion resistance. These properties arise from the behavior of the polymer matrix in the region near the filler phase, known as the interphase, where interactions between the polymer and filler phases lead to matrix properties that are modified from the bulk. At the interphase, polymer composite materials transfer load from the weaker matrix to the filler, thus enhancing mechanical properties. This makes tuning the properties of the interphase very important to composite performance.

In this study, we use molecular dynamics to study a system of polycarbonate (PC) chains confined between crystalline silica surfaces (alpha-quartz with hydroxy terminated end groups) to model how the presence of the surface effects structure and dynamics in the polymer material. The PC/crystalline silica surface system is built and initialized at a high temperature where the PC is a melt. From this high temperature, the system is cooled at specified cooling rates until it reaches a solid (glassy) state well below the glass transition temperature (Tg). We use different cooling rates, which affects the Tg of the PC, to create systems at the same low temperature with unique thermal histories for analysis. Between the high temperature liquid state and low temperature glassy state, density and mean-square displacement of the polymer are measured as a function of distance from the surface and compared to the values from bulk PC. From these measurements, we determine the distance from the surface where the polymer begins to behave via dynamics or density like the bulk material, thus defining the thickness and properties of the interphase region. Two different confinement thicknesses are also studied to study the effect of increasing gap size on the interphase size and dynamics.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Daniel Coile		
Academic Institution:	University of Maryland	**Major:** Biological Engineering
Academic Standing (Sept. 2021):	Sophomore	
Future Plans (School/Career):	Medical school	
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Material Science and Engineering, Polymers Processing Group	
NIST Research Advisor:	Dr. Tyler Martin	
Title of Talk:	Predicting Fluid Properties of an Embedded Ink 3D Print Using Machine Learning	

Abstract:

Embedded ink additive manufacturing uses a nozzle that prints ink into a support bath gel. Once printed and cured, the support bath is removed, leaving the ink structure. Although this type of additive manufacturing holds promise, it also has some drawbacks, namely, the properties of the fluids may cause the ink to bubble, air pockets to form, the filament to rupture, and other effects that would cause flaws in the print. In order to enable on the fly tuning of the print process, we developed machine learning tools to predict rheological properties of the fluids used in the print and support bath. Using simulations of embedded ink additive manufacturing, we applied image processing techniques to develop features from the simulated images. The resulting processed images were used as the training dataset for the ML estimators. These simulations used a range of ink and bath viscosities, including both Newtonian and Non-Newtonian fluids.

First we tried a variety of machine learning estimators to classify the type (Newtonian or Non-Newtonian) of fluid for the support bath and ink. Random Forest and Nearest Neighbor Classifiers performed the best on this task, acheiving 80% accuracy after some hyperparameter tuning. The regression estimators could then predict the viscosities of the bath and ink, if both were Newtonian fluids. In this case, the nearest neighbor regressor had a maximum r squared score of 0.999995. The simulation non-Newtonian fluids were Bingham plastics, which have a threshold yield, above which the material acts like viscous fluid, and below like a rigid body. The simulation images only display characteristics of the fluid post-yield, so moving forward we are attempting to predict the coefficients of the Herschel Bulkley equation which describes the nu of Bingham plastics. Future goals include training these estimators to experimental footage, and expanding the rheological properties predicted.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Maurice Curran		
Academic Institution:	University of Virginia	**Major:**	Chemical Engineering
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	I plan to have a career in chemical engineering.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Division HQ (Group 0)		
NIST Research Advisor:	June Lau, Alden Dima, Carelyn Campbell		
Title of Talk:	Natural Language Processing for Standardizing Vocabulary in an Electron Microscopy Schema		

Abstract:

In electron microscopy, many terms are used with similar meanings without a standardized dictionary for similar terms. For example, the phrases “high tension” and “accelerating voltage” both mean the same thing but are used in different research papers. This leads to significant accessibility and reusability problems within this community. The goal of this research is to develop a dictionary and a similarity score for “electron microscopy” terms using natural language processing. Using the Microscopy and Microanalysis conference abstracts as the raw data source, we used data from 2002 through 2019. Data preprocessing included isolating the bodies of the abstracts for analysis. The header information, references list, and DOI tags were placed in a different text file. A majority of the preprocessing was performed using spaCy (https://spacy.io/), an open-source software library for advanced natural language processing. The Matscholar (https://github.com/materialsintelligence/matscholar) API is an existing model for materials-focused natural language processing which was also used in analyzing the text files. This model was used to evaluate the types of keywords used in the research abstracts. The first phase of the project, preprocessing, has been completed. The group is now focusing on compiling the Matscholar tags and training a Gensim (https://radimrehurek.com/gensim/) word2vec model to evaluate the similarities of terms. The results of this research can be used to help in searching for related research terms within NIST and other scientific groups.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Daniel Delgado Cornejo		
Academic Institution: California Institute of Technology		**Major:** Physics
Academic Standing (Sept. 2021):	Graduated Senior	
Future Plans (School/Career):	Energy Sustainability Researcher	
NIST Laboratory, Division, and Group:	MML Mechanical Performance Group	
NIST Research Advisor:	Dr. Adam Creuziger	
Title of Talk:	Modeling Crystallographic Texture from Specific Pole Figures	

Abstract:

Crystallographic texture is an important property of material science which bridges the meso/microscale of physics to the macroscale of conventional engineering and technology. It describes the alignment of crystal orientations within a sample and can be modelled using an orientation distribution function (ODF). In order to construct these ODFs, we can use some combination of pole figures (PFs) which can be found empirically from x-ray diffraction or neutron diffraction techniques. However, it is not intuitive if all pole figures are equally valuable to construct the ODF. Each PF yields incomplete information of the crystal orientations, taken along a particular crystal plane. Continued study of ODF reconstruction raises further questions which we explore: how many PFs are needed to accurately construct an ODF? Which ones are better to use? How does the completeness, the crystal planes, and the scanning method of the PF affect the ODF reconstruction?

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Katherine Dura

Academic Institution: University of Maryland

Major: Bioengineering

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): I plan to attend graduate school at Duke University in Computational Biology and Bioinformatics.

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

NIST Research Advisor: Christina Bergonzo and Robert Brinson

Title of Talk: Assessing Structural Effects of RNA Modifications in Molecular Dynamics Simulations

Abstract:

RNA has many uses in clinical applications such as siRNA therapies or vaccines, becoming more commonly known with the COVID vaccine. One major issue with using RNA is the inherent instability of the molecule, but the structure of the molecules can be modified to allow the RNA to remain stable for longer periods of time. Molecular dynamics, using the AMBER software package, was used to compare the dynamics of the selectively modified NIST siRNA to unmodified RNA. Atomic positions and fluctuations were evaluated through analysis metrics including base pairing, helical structure, and sugar puckering. When modifications were made to only the 7th residue, no differences were observed for RMSD, RMSF, base pairing, nor helical structure. However, the modifications to residues 6, 7, and 8 together appeared to produce substantial structural changes. These results indicate that there is a minimum number of modifications that will be needed to change the dynamics of the RNA molecule, but that the stability can be affected by adding functional groups. Simulations such as this one might be used in the future to predict the effect of modifications to RNA and to modify molecules in more specific ways.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Jalen Garner			
Academic Institution:	Howard University	**Major:**	Physics
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Graduate School (MS/ Ph.D. Dual)		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Group 642.05		
NIST Research Advisor:	Francesca Tavazza		
Title of Talk:	Effect of Mechanical Strain on the Electronic and Magnetic Properties of UTe2		

Abstract:

Unconventional superconductors have challenged current experimental and theoretical understandings of superconductivity, leading to an emergent research path for quantum materials science. Recently, Uranium-based compounds such as UGe2, UReGe, and UCoGe, have been studied due to their wide range of physical attributes. Among them, a newly rediscovered unconventional superconductor, UTe2 has attracted large attention due to evidence of the spin-triplet state and magnetic phase transitions under external magnetic fields. U-based superconductors are challenging for traditional density functional theory (DFT) electronic structure methods due to the unphysical electron self-interaction that tends to delocalize the d & f orbitals. The DFT+U method helps correct this error by imposing a penalty on partially occupied orbitals, encouraging localization, and improving the electronic structure. However, the value of U has to be determined on a case-by-case basis. Using first-principle calculations, in this work, we screened for an appropriate exchange-correlation function and U parameter to reproduce known electronic structure characteristics of the material. We then used such a model to identify the UTe2 magnetic ground state. Continuing this work, the selected computational parameters will be used to probe the mechanical properties and band structure of UTe2 as a function of tensile and compressive strain. We hope our work will provide guidance about how to tune the properties of UTe2 using mechanical strain.

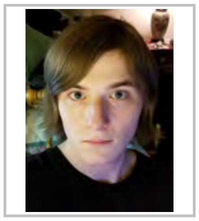
SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Wyatt Gibbs		
Academic Institution:	Salisbury University	**Major:**	Chemistry
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Graduate Studies for Chemistry/Materials		
NIST Laboratory, Division, and Group:	MML, Materials Science and Engineering Division, Polymers Processing Group		
NIST Research Advisor:	Dr. Peter Dudenas		
Title of Talk:	Procedural Polymer Morphology Generation for Resonant Soft X-Ray Scattering Simulations (RSoXS)		

Abstract:

Developing robust structure-property relationships in organic semiconducting materials is crucial to enable cheap, light-weight, and flexible organic electronic devices such as organic field-effect transistors (OFETs), organic solar cells (OPVs), and organic based displays. Resonant soft x-ray scattering (RSoXS) has recently begun to establish itself as a powerful tool for understanding these materials because of it's sensitivity to both crystalline and non-crystalline molecular orientation. Thus, it has the ability to characterize morphology in more detail than non-resonant scattering or electron microscopy techniques. However, careful interpretation of experimental RSoXS data typically benefits from supporting scattering simulations. Here, we present tools to procedurally generate morphologies/systems for use in our forward scattering simulator (Cy-RSoXS) and apply them to a model system of Poly[2,5-bis (3-tetradecylthiophen-2-yl)thieno[3,2-b]thiophene] (PBTTT), a popular high-mobility semiconducting polymer. The resulting Cy-RSoXS simulations of coarse-grained PBTTT morphologies are expected to fit experimental RSoXS profiles, and scattering energy dependence previously established in literature. Fitting experimental data in this context provides a deeper understanding of features in RSoXS data and the parameters that define them. Generalization of this approach is likely able to find significant utility in other related morphologies/systems.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Catherine Gill

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

Academic Standing (Sept. 2021): Graduated

Future Plans (School/Career): Take part in a post baccalaureate program at NCI-Frederick before pursuing a doctoral degree.

NIST Laboratory, Division, and Group: Material Measurement Laboratory

NIST Research Advisor: Dr. Christina Bergonzo

Title of Talk: Understanding the Importance of The Peptide Chain in Representatively Modeling teClpS Binding Preference.

Abstract:

ClpS2 is a small protein in the bacterial N-terminal degradation pathway where it binds other proteins before directing them to the ClpAP complex for degradation. ClpS2's unique binding is based on the identity of the N-terminal amino acid of the protein it binds, making it uniquely qualified for use as a reagent in next generation protein sequencing methods. Thermosynococcus elongatus derived ClpS2 (teClpS) is unique as it has been shown in bench analysis to preferentially binds to leucine, a non-aromatic non-polar amino acid, while most other ClpS2 proteins preferentially bind aromatic amino acids (such as Tyrosine, Phenylalanine, and Tryptophan). Previous Molecular Dynamics (MD) simulations of teClpS2 bound to single NAA ligands have so far been unable to replicate this trend. To better understand this discrepancy, and develop a more robust model for future analysis, we used MD simulations to characterize the differences in binding between a three-residue peptide and single NAA forms of bound ligand. We validate our model against solution state experimental data, to determine how accurately this peptide ligand model represented real world interactions.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Devin Golla		
Academic Institution:	Columbia University	**Major:**	Chemical Engineering
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Graduate studies in Chemical/Biomedical Engineering		
NIST Laboratory, Division, and Group:	MML, Materials Science and Engineering Division, Polymers and Complex Fluids Group		
NIST Research Advisor:	Robert Ivancic		
Title of Talk:	Modeling the Structure-Property Relationships of Diblock Copolymer Architectures		

Abstract:

Diblock copolymers of polyethylene and linear low-density polyethylene are promising candidates for compatibilizers to increase the structural integrity of recycled polyolefin composites. In this work, we studied the relationship between the architectures and the dilute solution properties of these copolymers. To do this, we simulated a coarse-grain, implicit solvent molecular dynamics model in which interactions between monomers were governed by a force field designed to replicate experimental dilute solution properties in a good solvent. For each architecture we modeled, we used the ZENO code to calculate its radius of gyration, intrinsic viscosity, and hydrodynamic radius. We then observed how varying the molecular weight, branch length, and relative polyethylene composition changed these properties. Consistent with experiments and theoretical predictions, we observed power law scaling between molecular weight and dilute solution properties for all studied polymer architectures. At constant molecular weight, these properties decreased as branch length increased, and increased as the percentage of polyethylene in the diblock increased. We related changes in these properties to the backbone and persistence length of our polymer chains, providing a physical rationale for these changes. These findings add to a library of novel polyolefin architectures and their dilute solution properties, providing valuable clues to develop a broader theory connecting polymer structure to properties in good solvents. More narrowly, these results provide useful benchmarks for experimentalists designing diblock copolymers of polyethylene and linear low-density polyethylene for use as compatibilizers.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Eleanor Grosvenor		
Academic Institution:	University of Maryland, College Park	**Major:**	Materials Science and Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	PhD in Materials Science and Engineering		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Functional Nanostructured Materials Group		
NIST Research Advisor:	David Raciti		
Title of Talk:	Computational Modeling of Commercial CO2 Electrolyzers Equipped with Nanostructured Cathodes		

Abstract:

Carbon dioxide emissions are the leading cause of anthropogenic climate change. To combat this issue, we can use electrochemical CO2 reduction, a method of carbon utilization in which electrolyzers convert CO2 gas to CO for fuel. The durability of commercial high-flux electrolyzers can be improved by supporting a conductive catalyst layer (CL) network on a non-conductive, porous gas diffusion layer of polytetrafluoroethylene. In our work, we selected high aspect ratio Ag nanowires because their 1-D structure enables the creation of a porous CL. The high surface area of the nanostructured CL increases CO2 flux and conversion at the working electrode, but also leads to complex interactions among the catalyst surface, electrolyte, and gas species. To better understand these interactions, we built a 1-D computational model in COMSOL to explore the microenvironment limitations during electrochemical CO2 reduction. We used the model to predict the conditions of the catalyst microenvironment within a series of varying catalyst layer thicknesses using two electrolytes, KHCO3 and KOH. High alkalinity electrolytes like KOH have demonstrated high activity for CO2RR, but also maintain high local concentrations of hydroxide. The model predicts that excess hydroxide consumes CO2, competing with electrochemical CO2 conversion and producing carbonate at high concentrations, both processes being detrimental to sustained electrolyzer efficiency. Seeking to further our understanding of the dynamic interplay between hydroxide and dissolved CO2, we are in pursuit of modeling the complex gradients that likely exist in the catalyst layer via a 3-D construct that takes into account the porosity and physical interactions of the gas molecules. This model will give more insight into the optimization of electrochemical CO2 reduction with respect to electrolyzer efficiency.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Ross Gunther

Academic Institution: Georgia Institute of Technology

Major: Materials Science and Engineering

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Work as a materials engineer

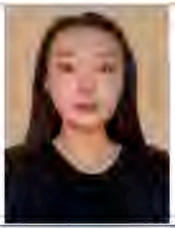
NIST Laboratory, Division, and Group: Materials Measurement Laboratory, Materials Science and Engineering Division, Polymers Processing Group

NIST Research Advisor: Leanne Friedrich

Title of Talk: Maximizing Cell Viability in Embedded 3D Bioprinting

Abstract:

Additive manufacturing, where objects are made by layering material upon itself, enables engineers to create objects which are impossible using conventional fabrication techniques. Embedded 3D printing is a type of additive manufacturing where instead of layering material in air, fluid inks are deposited into a support fluid. This allows for printing using soft materials which would collapse with other techniques. Embedded 3D printing is notably useful for printing live tissue. A bioink is created by mixing tissue cells with a carrier material which protects the cells and provides nutrients. A major concern is that when bioinks are ejected from the printer nozzle, they are subject to high shear stresses which are detrimental to cell health. By changing the nozzle shape from cylindrical to conical, shear stress on the bioink should be reduced which will lead to greater cell viability. We confirmed this hypothesis using OpenFOAM, a computational fluid dynamics simulator. Models of a 3D printing chamber, including nozzles, fluids, and housing structures, were generated using Python and read into OpenFOAM. The simulations show that as the nozzle angle increases, the number of cells affected by high shear stress decreases. Interestingly, the maximum shear stress for a select few cells increases as nozzle angle increases as well. This means that a few cells incur higher adverse effects from the printing process. However, this is of minimal consequence because the greater quantity of healthy cells will reproduce to replace these few cells. Overall, this research found that it is advantageous to use a 20 degree angled nozzle for embedded 3D bioprinting because it minimizes high shear stress while minimally compromising print quality. These findings promote embedded 3D printing as a promising fabrication technique for bioprinting. This novel fabrication technique can be applied to reconstruct veins, ligaments, and eventually even organs.



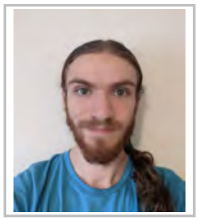
SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Bliss Han		
Academic Institution:	Brown University	**Major:**	Environmental Science
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Pursuing a graduate degree or a career in environmental science		
NIST Laboratory, Division, and Group:	Material Measurements Laboratory, Chemical Sciences Division, Chemical Informatics Group		
NIST Research Advisor:	Nathan Mahynski		
Title of Talk:	Understanding Self-Assembly of Programmable Polycrystalline Films		

Abstract:

Self-assembling two-dimensional DNA-based frameworks are crucial to nanoscale engineering. The self-assembly of these structures is important because it is difficult to manually assemble large, meter-scale structures out of nanometer-scale objects. Thus, these structures must be chemically programmed to assemble themselves via thermodynamics. The intent of this project was to explore how mathematical concepts of symmetry, specifically those related to planar tilings and tessellation, can be used to better understand how these patterned surfaces can be programmed to self-assemble. The fundamental domain of a crystal is an isohedral tile, and the two-dimensional structure formed by the self-assembly of these domains can be considered an isohedral tessellation. The Heesch System for classifying isohedral tiles which tessellate two-dimensional Euclidean space, where tiles are identified by the symmetries of their edges - Translation (T), Glide Reflection (G), and Rotation (C) - was expanded to include reflection symmetry (A). This new rational naming scheme was used to characterize all 93 isohedral tiles. These tiles were used to further explore how correct self-assembly is made possible by curving the edges of the tiles, as tiles with straight edges can form defective structures which do not tessellate. Since the 93 isohedral tilings represent every single two-dimensional periodic pattern, this classification system provides a theoretical framework that allows engineers to easily and rationally build fundamental domains that can self-assemble into two-dimensional nanostructures with various technical applications.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Noah Hobson			
Academic Institution:	University of Tennessee, Knoxville	**Major:**	Computer Science
Academic Standing (Sept. 2021):	Graduated Student		
Future Plans (School/Career):	Ph. D. at Purdue University		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory; Office of Data and Informatics; Data Sciences Group		
NIST Research Advisor:	Gretchen Greene and Raymond Plante		
Title of Talk:	Applying Natural Language Processing to the NIST Public Data Repository		

Abstract:

NIST manages a growing collection of free to use data records for the general public called the NIST Public Data Repository. The NIST Science Data Portal is the user gateway where the records in the repository can be searched through using free text entry of keywords, names, research topics and user provided subject matter. To facilitate search through this complex data space on a particular subject, a taxonomy of common words and phrases is created using Natural Language Processing to create meaningful connections within word phrases, combined with traditional keyword matching using the authors' manually written keywords. Different methods are combined to produce the most optimal search suggestions, which appear as a user types, and fuzzy selection is employed to match potentially misspelled or related terms to help guide users toward what they are looking for. The Natural Language Processing algorithm used for the Science Data Portal's taxonomy is also applied to the Brookhaven National Laboratory's database of quantum science abstracts in collaboration with the Co-design Center for Quantum Advantage (C2QA) data working group. The generated semantic output will be used to prototype domain specific taxonomy to determine popular terms for tagging quantum research publications. This is done as a proof of concept for the algorithm's performance beyond the original scope of the project, and to explore how well it generalizes to both multi-disciplinary and domain specific application.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Jordan Hoffman

Academic Institution: University of New Hampshire

Major: Mechanical Engineering

Academic Standing (Sept. 2021): First-year graduate student

Future Plans (School/Career): Pursue Master of Engineering in Mechanical Engineering from the University of New Hampshire

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Materials Science and Engineering Division, Center for Automotive Lightweighting

NIST Research Advisor: Dilip Banerjee and Mark Iadicola

Title of Talk: Determination of Strain Path Envelope in an Optimized Cruciform Specimen of AISI 1008 Steel

Abstract:

The automotive industry relies heavily on the sheet metal forming process for many components. The material data currently available, from uniaxial testing, is insufficient and results in long trial and error periods and frequent unpredicted failures. Biaxial cruciform testing is a better representation of the forming process than traditional uniaxial testing since sheet metals are anisotropic, but this testing requires special geometries to reach various biaxial strain combinations. Using a previously optimized specimen for AISI 1008 steel, the strain path envelope and the required displacement control could be determined through numerical simulation in Abaqus 2019, a finite element analysis software. Linear biaxial displacements were applied to the specimen with the goal of observing a linear strain path. While the strain paths produced were not linear, the results could be used to reverse engineer a new displacement path that would produce a linear strain path. Systematic adjustments were made to determine the new displacement path utilizing Isight (an optimization software), incremental adjustments, and interpolation from the linear displacement path results. These methods of linearizing the strain path could then be applied to bilinear simulations, which approximate a two-stage forming process. The biaxial simulations included test conditions that begin in uniaxial and transition to equibiaxial, as well as conditions that begin in equibiaxial and finish in a plain strain condition. Performance of these studies entailed creating a Python code to post-process FEA computed average strain data in the gauge area, executing mesh quality enhancement and mesh sensitivity studies, checking element type and strain-rate material model dependencies, as well as the dependency of total step time. Thorough analysis of the simulation results shows that a linear strain path of a given model can be determined utilizing the strain data from an applied linear displacement path.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Jesse Ji			
Academic Institution:	Northwestern University	**Major:**	Mechanical Engineering and Biology
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Pursue a career in the aerospace industry.		
NIST Laboratory, Division, and Group:	Material Measurement Laboratory, Materials Science and Engineering Division, Thermodynamics and Kinetics Group		
NIST Research Advisor:	Carelyn Campbell		
Title of Talk:	Modeling Creep in Co-based Superalloys with AI		

Abstract:

Superalloys are alloys that exhibit good mechanical strength and creep (deformation) resistance at high temperatures, and they are extensively used in the aerospace and energy industries, having applications in aircraft engines, turbines, and nuclear power plants. Nickel-based superalloys are conventionally used over cobalt-based superalloys due to their superior strength, but the implementation of precipitate-strengthening of Co-based superalloys has introduced a novel class of alloys with similar strength to that of Ni-based superalloys, the γ/γ' Co-based superalloy. The higher solidus and liquidus temperatures of these alloys mean that they can be operated at higher temperatures, and thus, show greater efficiency and performance.

This project focuses on utilizing machine learning techniques to model creep behavior in Co-based superalloys as a function of alloy composition with the goal of designing the optimal Co-based superalloy to maximize creep resistance. An effective machine learning algorithm would prove to be advantageous as it eliminates the time and resources needed for the synthesis and testing of each individual alloy.

Modeling of creep behavior in this project is based on a regression model for creep-rupture life that depends on the parameters of lattice misfit and γ' phase volume fraction. The values for these parameters were obtained from both experimental data in literature and from CALPHAD-generated data for 800+ Co-based alloys of varying compositions of cobalt, nickel, aluminum, tungsten, titanium, tantalum, and chromium. The compiled data will be used to train various machine learning models, the accuracy of which will be evaluated by their performance on a test set of data.

	# SURF Student Colloquium NIST – Gaithersburg, MD August 2-6, 2021

Name:	Jennifer Li		
Academic Institution:	University of Maryland, College Park	**Major:**	Neuroscience and Information Science
Academic Standing (Sept. 2021):	Sophomore		
Future Plans (School/Career):	Pursue a MD-PhD dual degree in medicine and research		
NIST Laboratory, Division, and Group:	MML, Biosystems and Biomaterials Division, Cell Systems Science Group		
NIST Research Advisor:	Elijah Petersen		
Title of Talk:	Evaluation of Carbon Nanomaterial Bioaccumulation Studies and Methods		

Abstract:

Environmental pollution is becoming an increasingly important issue. For example, particulate substances from products in the environment have the potential to bioaccumulate in organisms that intake such compounds. One key type of particulate substances are carbon nanomaterials such as nanoplastics, carbon nanotubes, fullerenes, and graphene family materials. A wide range of techniques have been utilized to research bioaccumulation of carbon nanomaterials, as well as trophic transfer of compounds to other organisms. In this project, bioaccumulation studies were critically evaluated in order to analyze the validity and applicability of the methods used.

These studies were characterized by the analytical method and year in order to understand trends in techniques used over time. In addition, studies were individually reviewed to extract important information including type and size of carbon nanomaterial, experimental setup, method, and relevant findings.

This review found that certain methods of evaluating bioaccumulation in organisms were more common for specific types of carbon nanomaterials. Some of the more frequently used techniques were carbon-14 labeling, transmission electron microscopy, and fluorescence. Overall, there was some uptake of nanomaterials by plant and other multicellular organisms. There was limited uptake of carbon nanotubules, graphenes, and fullerenes, while many studies focused on nanoplastics found uptake and absorption across epithelial surfaces. However, key control experiments were not performed for many of the nanoplastic studies which lowers confidence in these results.

This project demonstrates the importance of critically evaluating studies and corresponding methods, since the methodological details used could skew results. Strategies such as using control experiments are important to confirm the validity of methods used. Bioaccumulation and trophic transfer have the potential to affect large groups of organisms and food chains, making this a significant area of research.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Richard Ma

Academic Institution: University of California, Berkeley **Major:** Materials Science and Engineering

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate school/pursuing PhD

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group

NIST Research Advisor: Howard Joress, Brian DeCost, Jason Hattrick-Simpers

Title of Talk: Use of Bayesian Inference to Plot Parameter Probability Distributions for High-Entropy Alloys

Abstract:

X-ray diffraction is a powerful analytical technique that, through creation of unique diffraction patterns, can be used to quantify the crystal structure of a material. As we generate a simulated diffraction pattern given a set of known parameters, we can determine the characteristics of the observed material by modifying the parameters in our model until the simulated diffraction data match the real data.

Conventionally, a least-squares method of determining the parameters is used. This method, however, is relatively slow and not as practical for large data sets. In this project, Bayesian inference is applied to the same end. Given a dataset and a set of unknown parameters with a known functional effect on the data, Bayesian methods can generate probability distributions for each parameter.

A Bayesian approach to refinement addresses several difficulties associated with traditional least-squares fitting, such as the expertise needed to manually adjust parameters for a good refinement and the possibility of falling into false minima if done wrong. Bayesian potentially requires less expertise (though it benefits from good prior distributions), and additionally performs more accurately in the calculation of confidence intervals. This acknowledgement of uncertainty is important as real data will always contain noise.

Although this method is widely applicable to the analysis of any structure, in this project we seek to examine high-entropy alloys- alloys with many different elements all present in stoichiometrically large proportions. These methods will serve as an effective tool to determine how the degree of order present in the structure changes with consideration to the various phases that the material may take. Better understanding of the phases and ordering behavior and thus the entropy of a material will improve our ability to work with it and understand it.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Daniel Matthew Markiewitz

Academic Institution: Cornell University **Major:** Chemical Engineering

Academic Standing (Sept. 2021): Graduate Student

Future Plans (School/Career): I will be pursuing a PhD at Massachusetts Institute of Technology.

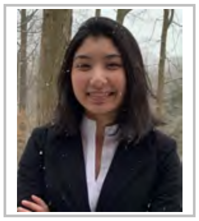
NIST Laboratory, Division, and Group: Material Measurement Laboratory, Chemical Sciences Division, and Chemical Informatics Group

NIST Research Advisor: Dr. Nathan Mahynski

Title of Talk: Designing colloidal crystals from functionalized polymer frameworks

Abstract:

All two-dimensional, periodic systems can be classified according to their crystallographic symmetry. There are 17 distinct symmetry, or wallpaper, groups for the Euclidean plane. The smallest “unit” of a crystal is its fundamental domain, or asymmetric unit, named because it does not contain any symmetry elements that operate on the unit to tesselate the plane. These groups may be described topologically as “orbifolds” which are essentially surfaces formed by folding the fundamental domain to match up symmetrically equivalent edges. Each wallpaper group has a unique orbifold and enumerating all ways to cut open the orbifold yields all topologically unique tiles that can tesselate the plane. There are 93 in total, defined by unique shapes and patterns along their edges. The mathematics required to understand these tilings have been studied exhaustively by many mathematicians, such as Heinrich Heesch and John H. Conway, and by artists such as M. C. Escher. This can be leveraged to program the self-assembly of nanoscopic objects by embedding them into a chosen tile whose shape and chemical functionalization program self-assembly into the corresponding wallpaper group. Another way to view this is as decoration of the colloid itself, which can be experimentally constructed via chemical modification of the colloid’s surface. Therefore, developing tools to assist scientists in using this orbifold-informed approach will enable a novel, rational design mechanism for programming colloidal self-assembly into bulk crystallographic lattices. In this project, we developed computational tools that simplify the colloid/tile design, which can then be exported to molecular simulation programs such as LAMMPS. We developed a graphical user interface that accomplished these goals by utilizing python and other native packages to minimize compatibility issues. This tool is expected to enhance engineers’ ability to utilize this rational design in their work, minimizing the resources needed for more computationally expensive iterative methods.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Miyu Mudalamane

Academic Institution: University of Delaware

Major: Chemical Engineering

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Attend graduate school

NIST Laboratory, Division, and Group: Materials Measurement Laboratory, Office of Data and Informatics, Data Sciences Group

NIST Research Advisor: Chandler A. Becker

Title of Talk: Demonstrating SciServer Applications for Additive Manufacturing Benchmark Data

Abstract:

The Additive Manufacturing Bench test series (AM-Bench) aims to provide the public with a comprehensive set of benchmark data that can be used to inform models of additive manufacturing processes. The tests are organized to address a series of “challenges,” providing data on the microstructure, strains, cooling rate, etc. of the materials used in the additive manufacturing process. SciServer, a collaborative web platform, can provide a platform for obtaining and working with AM-Bench data. It allows for researchers to collaborate closely on computational work, featuring cloud-based storage, shared folders, and a comprehensive query system. This eliminates many problems associated with hosting data locally, making it far easier to work with large datasets.

This project focuses on data from the 2018 AM-Bench tests - these datasets are publicly accessible, spread out over multiple databases. Within SciServer, sample datasets from the AM-Bench Configurable Data Curation System, or CDCS, instance (https://ambench.nist.gov) and the NIST Public Data Repository (https://data.nist.gov) were selected and their respective APIs were used to bring the data into the SciServer environment. The datasets selected for this project mostly involved measurements made as part of the melt pool characterization challenge. These images have clear-cut areas of interest, with a visible border between the melt pool and the rest of the metal tracks. As a result, image feature extraction algorithms could be used to isolate and measure area properties. Combining data from both databases, the measurements performed were compared to those obtained from related AM-Bench datasets. Correlations between laser speed, laser power, melt pool length, and melt pool depth were examined and graphed. Changes to the Python data processing and analysis scripts were tracked using Gitlab, mimicking a realistic workflow for a computational project. The results of this project can be used to demonstrate the capabilities of SciServer and facilitate its wider use throughout NIST for collaborative analysis.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Sareet Nayak

Academic Institution: University of Maryland, College Park

Major: Computer Science

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Industry (Bioinformatics)

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

NIST Research Advisor: Dr. Paul Salipante & Dr. Steve Kuei

Title of Talk: Modeling Flow Birefringence of fd-Virus Solutions through a Microfluidic Channel

Abstract:

Understanding how composition and structure of rod-like suspensions influence fluid properties is essential for research and pharmaceutical, personal care, and enhanced oil recovery applications. To study rod-like fluids' composition and structure, experiments in our lab use fd Virus as a model of rod particles due to its uniform length, stiff and monodisperse structure, and compatibility with theoretical models. The rheology and microstructure of rod-like fluids can be probed through various experimental techniques, such as capillary rheology and polarization imaging. We compute rod orientation and alignment in near-wall regions of our flow geometry using Computational Fluid Dynamics (CFD) to gain insight into these experimental results.

In this computational study, we use OpenFOAM, an open-source CFD software, to determine non-Newtonian fluids' behavior in straight channel flows, using several rheological models. In particular, we implement a rod-like constitutive model and its characteristic parameters that accurately define rod-like behavior at high shear rates. This model can then be utilized to describe flows in more complex geometries, such as entrance and cross-slot flows. Cross-validation between this experimental and computational system can provide a better understanding of rod-like fluids' microstructural dynamics and rheology and aid in the development of other suspension models.

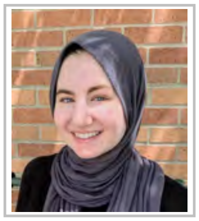
SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Anika Rajamani		
Academic Institution: Swarthmore College		**Major:** Computer Science, Applied Mathematics
Academic Standing (Sept. 2021):	Junior	
Future Plans (School/Career):	Pursue a career in AI/ML	
NIST Laboratory, Division, and Group:	MML	
NIST Research Advisor:	Dr. Talapady Bhat	
Title of Talk:	Developing R&R tools for AI	

Abstract:

Scholarly articles about COVID-19, SARS-CoV-2, and related coronaviruses from the COVID-19 Open Research Dataset (CORD) are stored and retrieved from the relational database system SQL Server. This project focuses on increasing the functionality of NIST's search tool that queries through the database and displays numerous representations of the requested data. I worked to implement a multi-term search tool that finds articles such that the abstract contains multiple user-inputted phrases. Additionally, the search tool verifies the preservation of the inputted phrase in the selected articles, assuring accurate results. Specifically, utilizing advanced SQL predicates including contains, near, inflection, and thesaurus allows us to perform a more sophisticated, complex search through the database. Further, C# object-oriented programming in Microsoft's Visual Studio Integrated Development Environment (IDE) was used to support the front-end development of the query tool. Rigorous speed and accuracy testing was performed on the page using the IDE's Internet Interface Services (IIS) feature to host ASP.NET web applications. Looking ahead, I will continue to build on the graphical and visual representations of this data and increase the efficiency of the application.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Malaak Saadah

Academic Institution: University of Illinois at Urbana-Champaign

Major: Materials Science and Engineering

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Graduate or professional school

NIST Laboratory, Division, and Group: Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Group

NIST Research Advisor: David Sheen

Title of Talk: High-throughput Machine Learning for Chemical Informatics

Abstract:

The goal of this project is to predict the bulk properties of fluids with minimum experimentation using machine-learning models. An important property to be calculated from the machine-learning model is compressibility, which is the deviation of a fluid's behavior from the ideal gas equation. Additional properties may be extrapolated if the compressibility of a fluid is known. By using the temperature, density, and information on virial coefficients as inputs to a machine learning algorithm based on adaptive-boosted neural networks, the compressibility of a fluid can be determined. The model is trained on the training set of several model fluids with different interaction potentials using a variety of neural network architectures. These architectures are obtained by changing the number of layers, neurons per layer, and number of adaptive boosting steps. Thus, the resulting machine learning algorithm will be able to predict the compressibility of new fluids, as long as the input data for those fluids are known. Once the compressibility of a fluid is calculated through this algorithm, it may be used to determine further properties such as entropy and enthalpy. Currently, the model gives good results for model fluids that are close to the training set, but extrapolation of the model to very different fluids does not result in good agreement with the test data. It was found that a single machine learning neural network model is not sufficient in predicting the compressibility of a diverse set of fluids. However, a model may be created to predict the properties of a given class of fluids.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Logan Saar		
Academic Institution:	University of Maryland, College Park	**Major:**	Materials Science & Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Pursue graduate degree in field of Materials Science & Engineering		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group (643.04)		
NIST Research Advisor:	Dr. Aaron Gilad Kusne		
Title of Talk:	Bayesian Analysis based Active Learning System for Autonomous Physical Science		

Abstract:

Autonomous physical science is a rapidly developing field, where artificial intelligence controls experiment design, execution, and analysis in a closed-loop to maximize the knowledge recovered from a limited number of experiments while simultaneously removing the need for continual human input. The field has superseded traditional Edisonian trial and error methods in its ability to reduce the number of experimental trials required to optimize target properties. However, there has not been a significant exploration into the concomitant recovery or discovery of meaningful models to explain fundamental physical trends potentially governing the data. The aim of this study is to incorporate closed-loop hypotheses testing via active learning methods to guide experimental setup, execution, and analysis. Updating the parameters of candidate physical explanatory models based on incoming data is the next step in autonomous physical science because it allows alteration of the experimental design to adjust for renewed inferences about the data. In this study, Bayesian analysis - in which the assigned likelihood of candidate hypotheses are updated after data acquisition - is employed to guide an autonomous liquid mixing robot in its search to recover the underlying law governing the pH of self-prepared buffer solutions. Candidate hypotheses are generated via symbolic regression methods and ranked by their likelihood in having generated the data. The efficiency and accuracy of this process in retrieving a proper model for the intrinsic law is investigated.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Priya Shah

Academic Institution: University of Pennsylvania **Major:** Bioengineering

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Graduate School or Career in Industry

NIST Laboratory, Division, and Group: Materials Measurement Laboratory, Materials Science and Engineering Division and the Office of Data and Informatics, Data Sciences Group

NIST Research Advisor: June Lau and Gretchen Greene

Title of Talk: Research and Development of the NexusLIMS

Abstract:

The Electron Microscopy Nexus is a network of microscopes that facilitates materials science research. Presently at NIST, there is a workflow engine called NexusLIMS which handles basic capturing of electron microscopy observation sessions. Captured images and metadata generated by the microscope from each microscopy session are stored and available for search and preview on the web directory. This project seeks to augment the capabilities of the current workflow engine to associate additional data, such as corresponding electronic lab notebooks, to the observational data. In parallel, the project investigates on-cloud computing capabilities with which researchers could view and analyze experimental observations and associated data without saving each file to their individual workspace.

For electronic lab notebooks developed in Microsoft OneNote, the content of a relevant notebook is captured using Microsoft Graph API. The textual content of each page of the notebook is saved as an HTML file that will later be accessible and associated with the corresponding captured images and metadata through NexusLIMS. Non-textual content of an electronic lab notebook page, such as images and InkML content, is obtained and saved under a descriptive name for ease of access. Providing the notes associated with observational data to researchers who hope to expand upon or replicate results of another experiment gives those researchers important information about expected results, experimental processes, and other aspects of the experiment.

For researchers working on expanding or replicating the results of another experiment, the ability to easily search and access files associated with an experiment is important. This project is working on developing methods of querying of the NIST Configurable Data Curation System and analyzing the returned data within the browser, without requiring users to download the returned data files in order to analyze them.

We hope to connect these changes to the current workflow engine to create a searchable resource for researchers that includes content from electronic lab notebooks and enables on-cloud computing. We hope these augmentations to the current workflow engine, in tandem, will allow for a heightened ability for researchers to collaborate and replicate scientific results of their peers. Such abilities would enable further electron microscopy data discovery and long-term management of observed and analyzed data.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Michaela Staab	
Academic Institution: University of Maryland	**Major:** Bioengineering
Academic Standing (Sept. 2021):	Junior
Future Plans (School/Career):	Graduate School
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory
NIST Research Advisor:	Curtis Meuse
Title of Talk:	Data Analysis Methods to Describe Molecular Conformational Ensembles

Abstract: Proteins are large molecules that exist as mixtures of both atomic compositions and peptide backbone configurations. The pharmaceutical industry and regulatory agencies require information describing the molecular members of these mixtures to improve the efficacy and safety of protein-based drugs. Infrared (IR) spectroscopy is a rapid method for characterizing proteins and protein-based drugs. While IR spectroscopy does not typically measure subpopulations, it can measure protein concentration, observe protein aggregation, quantify protein stability, and compare the secondary structures of proteins in solution. These capabilities, as well as IR spectroscopy's high sensitivity to water, potentially allow for the development of techniques to measure the IR spectra of protein subpopulations.

The goal of this project is to use multivariate curve resolution techniques to unmix the IR spectra of subpopulations due to the interactions between proteins and water from the spectral contributions of other populations. Data will be collected with different concentrations of water and protein and at different rates of water evaporation. These data will be analyzed by performing multivariate curve resolution – alternating least squares to determine the spectra and fractions of the subpopulations present.

The ability to separate the spectra of the subpopulations provides a path to clarify the identities of the members of the mixtures and their relative concentrations. This project has begun to tackle the differentiation of the spectra and the determination of the number of target subpopulations. This information could be critical to the pharmaceutical industry as the disparate subpopulations of protein drugs could have different potencies.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Chloe Taylor

Academic Institution: Harvey Mudd College **Major:** Physics

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Attend Graduate School

NIST Laboratory, Division, and Group: Materials Measurement Laboratory, 642, Functional Nanostructured Materials

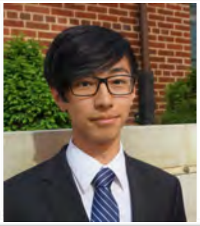
NIST Research Advisor: Daniel Gopman

Title of Talk: Large Interlayer Exchange Coupling in Ir-based Synthetic Antiferromagnets

Abstract:

The synthetic antiferromagnet (SAF) is a functional nanostructured material comprising two or more thin ferromagnetic layers separated by a nonmagnetic layer. An interlayer exchange coupling between the separated layers produces the antiparallel (or parallel) alignment of the ferromagnet layers. SAFs are used in magnetoresistive random-access memory (MRAM) to fix the orientation of a reference magnetic layer in the memory device. Industry is interested in SAFs comprising a Co/Pt multilayer –bilayer repeats of Co and Pt, each of sub-nm thickness – with a sub-nm Ir insertion to convey an antiferromagnetic exchange energy exceeding 2 mJ/m2 – enough to maintain the anti-parallel orientation of the SAF layer in the memory device. This figure of merit does not meet or exceed any theoretical limit, so we sought to develop advanced processing methods to increase the exchange energy.

The Magnetic Engineering Research Facility can produce SAFs with precise control over interfaces and sub-nanometer thickness employing direct current magnetron sputtering, a physical vapor deposition technique. We examined SAFs with Co/Pt ferromagnetic layers split by an Ir spacer layer. Specular x-ray reflectivity was used to precisely calibrate the thicknesses of test samples using Argon, Krypton, or Xenon as the ionized gas for sputtering the Co (Pt, Ir) targets. Our deposition rate calibrations informed the growth of SAF samples with a laterally varying Ir layer, using Argon, Krypton, or Xenon gas. The interlayer exchange coupling field, saturation magnetization, and magnetic anisotropy field were measured using a vibrating sample magnetometer (VSM). We found the figure of merit for a SAF, the interlayer exchange coupling energy, to be greatest overall for the Xe sample, followed by Kr and then Ar, with an increase of over 30% for the Xe sample compared to the state-of-the-art. This highlights the importance of magnetic materials processing to advance the materials performance for memory devices.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	**Alex Wang**		
Academic Institution:	University of Maryland, College Park	**Major:**	Materials Science & Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Pursue a career in Computational Materials Engineering and go to graduate school.		
NIST Laboratory, Division, and Group:	Materials Measurement Laboratory, Materials Measurement Science Division, Materials for Energy and Sustainable Development Group		
NIST Research Advisor:	Aaron Gilad Kusne		
Title of Talk:	Benchmarking Active Learning Strategies for Materials Optimization and Discovery		

Abstract:

Autonomous physical science has the ability to revolutionize how materials science is performed. Compared to traditional materials discovery strategies, algorithmically searching materials systems for optimal materials reduces the time and cost of experiments by optimally collecting knowledge-rich data. Such an approach is becoming ever more popular with developments in active learning and scientific AI. We present a benchmarking study to compare the efficacy of popular off-the-shelf active learning methods and those designed with incorporated knowledge of the materials optimization challenge. In this study we benchmark active learning strategies on 5 ternary composition materials datasets containing composition, structure, and functional property data and evaluate the impact of prior knowledge on materials optimization.

NIST Center for Neutron Research (NCNR) Participants

Owen Bailey

Claire Lamberti

Kate Meuse

Sidney Molnar

Jessica Opshal-Ong

Patrick Park

Ryan Puthumana

Jack Rooks

Daven Shah

Aurora Zemborain

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Owen Bailey

Academic Institution: Bates College

Major: Chemistry

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Pursue a Ph.D. in Chemistry, focusing on Materials Chemistry solutions to environmental problems.

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

NIST Research Advisor: Dr. Hayden Evans

Title of Talk: Organic Cation Dynamics of Hybrid Vacancy-Ordered Perovskites $(FA)_2PtI_6$ and $(GA)_2PtI_6$

Abstract:

Current research into halide perovskites with the formula AMX_3 is focused on improving their functionality in high-efficiency thin-film, single-junction photovoltaic devices. These AMX_3 materials, where A is an alkali-metal or small organic cation, M is a divalent main group metal, and X is a halide, demonstrate excellent optoelectronic properties and notable ease of preparation. Unfortunately, these materials are sensitive to external factors, namely their instability in air. To alleviate this instability, research into perovskite-related materials has expanded to include hybrid vacancy-ordered perovskites, where a trivalent M site ion forces every third M to be missing, or where a tetravalent M site ion creates vacancies and (usually) displays a rock-salt-like ordering. Unlike traditional AMX_3 compounds, hybrid vacancy-ordered perovskites are impacted by the organic A site cation which can ultimately determine the compound’s performance.

One such example, formamidinium Sn(IV) iodide, $(FA)_2SnI_6$, displays a ferroelastic phase transition driven by organic–inorganic coupling. To understand if this phase transition is ubiquitous in vacancy-ordered systems, we are analyzing the isostructural hybrid A_2PtI_6 compounds formamidinium platinum iodide, $(FA)_2PtI_6$, and guanidinium platinum iodide, $(GA)_2PtI_6$. Our research will focus on these two compounds, as we utilize quasielastic neutron scattering (QENS) and X-ray powder diffraction to analyze the dynamic nature of the organic cations in the compounds as they vary in temperature and undergo phase transitions. QENS data collection will take place at Oak Ridge National Laboratory’s Backscattering Silicon Spectrometer, and X-ray diffraction data will be collected through the Advanced Photon Source’s 17-BM-B.

Through our analysis we hope to establish synthetic guidelines to inform future development of new materials in this class of compounds, namely how to view certain commonly used organics and their potential to change structures in predictable ways.

SURF Student Colloquium

NIST – Gaithersburg, MD August
2-6, 2021

Name: Claire Lamberti

Academic Institution: University of Texas at Tyler

Major: Chemistry and Physics

Academic Standing (Sept. 2021): Southern Methodist University - First Year Graduate Student

Future Plans (School/Career): Attend graduate school pursuing a PhD in Physical Chemistry

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

NIST Research Advisor: Dr. Craig Brown

Title of Talk: Broad-Spectrum Antibiotic Glasses with Tunable Solubility

Abstract:

The World Health Organization (WHO) maintains the Model List of Essential Medicines. This list contains the medications considered to be most effective and safe to meet the most important needs in worldwide health systems. Many of the essential drugs on this list suffer from poor aqueous solubility, which affects their bioavailability and renders them less effective. Typical strategies to improve the physicochemical properties are the formation of polymorphs, salts, cocrystals, and amorphous formulations. In this regard, we face a major challenge: in many cases, the crystal structure of the drugs is unknown. A common culprit for the lack of crystallographic knowledge is the fact that many of these drugs do not crystallize as single crystals but form polycrystalline powders. Here, we collected powder X-ray diffraction pattern of a prominent member of the WHO list. Our next steps are collection of powder neutron diffraction patterns, and solution of the crystal structure. The rise of multi-drug resistant bacteria, and new diseases and pathogens, demand the development of more advanced strategies to control the pharmaceutical solid-state, beyond polymorphism, salt formation, co-crystallization and amorphization. Here, we decided to develop a new and bold strategy to control the solid-state structure—we stabilize medicine in the form of a glass. We provide proof-of-concept that a prominent member of the WHO list can be glassified, as evidenced by the visual appearance, and the glass transition in the calorimetric curves. The molecular structure is unaltered, and the molecule can be easily released in aqueous solution, as evidenced by the nuclear magnetic spectra. By careful combination of different molecules in the glass, we managed to achieve chemical reaction between the drugs into a new drug-based peptide. This peptide material is also glassy and does not dissolve in water. Finally, by controlling the degree of peptization, we can control the overall solubility of the glass. The next steps in our research are deciphering the local structure of the glass material. In this regard, neutron-based methods are of extreme importance. I will present our preliminary data, and I will outline a research strategy how to better understand these broad-spectrum antibiotic glasses with tunable solubility.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Kate Meuse
Academic Institution:	Cornell University
Major:	Computer Science
Academic Standing (Sept. 2021):	Sophomore
Future Plans (School/Career):	Finish BS, possibly MEng, then work in industry
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group
NIST Research Advisor:	William Ratcliff
Title of Talk:	Classifying Spin-Interactions using Reinforcement Learning

Abstract:

Every year, the NIST Center for Neutron Research receives more beam time applications than it can grant. Neutrons come at a premium, with only a handful of scattering facilities in the US, so every measurement should be optimized. One such measurement is the determination of magnetic structures within a crystal lattice. We approximate the energy of spin interactions using a Heisenberg Hamiltonian, which, when minimized, provides the ground state for magnetic spin ordering. However, to uniquely derive the interactions that create the ground state, we excite the system with neutrons to create a spin-wave. From the measurement of this spin-wave, we can fit parameters of the Hamiltonian, namely the pair coupling matrices which describe the strength of interactions between spins.

In order to find these values efficiently in an experimentally efficient way, we employed OpenAI's plug-and-play reinforcement learning algorithms. The agents select useful vectors to scan along in reciprocal space to run a spin-wave measurement on while avoiding over-measurement. The goal was to reduce measurement times while classifying the underlying interactions in the magnetic structure. We expect to test multiple reinforcement learning algorithms on this problem to compare their relative effectiveness in this action space.

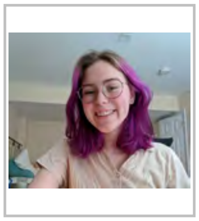
SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Sidney Molnar		
Academic Institution:	Hamilton College	**Major:**	Physics/Mathematics
Academic Standing (Sept. 2021):	Senior at Hamilton College		
Future Plans (School/Career):	Attend Graduate School to Receive a Masters Degree for Mechanical or Aerospace Engineering		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Wangchun Chen		
Title of Talk:	Optimizing a Magnetically Shielded Solenoid for Extended-Q SANS Polarization Analysis Capability		

Abstract:

We optimized the magnetic field gradient for a 3He neutron spin filter used to extend the Q range in polarized neutron measurements. Experiments using the 30m small-angle neutron scattering (SANS) and very small-angle neutron scattering (vSANS) instruments with polarization analysis at the NIST Center for Neutron Research contribute to research into small length scale nanomagnetism. In our spin filter, a 3He cell is polarized offline by spin-exchange optical pumping and stored in a magnetically shielded solenoid. The solenoid is then placed in a neutron beam where the spin dependence of the 3He cross section is used as a neutron analyzer. In order to extend the polarization lifetime of the spin filter, we optimized the uniformity of an asymmetric mu-metal shielded solenoid using two end compensation coils. Radio frequency (RF) coils were added to act as a spin flipper using the adiabatic fast passage (AFP) nuclear magnetic resonance (NMR) technique.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Jessica Opsahl-Ong			
Academic Institution:	Rice University	**Major:**	Computer Science
Academic Standing (Sept. 2021):	Sophomore		
Future Plans (School/Career):	Finish undergraduate, get a masters, work in industry		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	William Ratcliff		
Title of Talk:	Optimizing neutron scattering measurements to best determine spin interations in magnetic lattices		

Abstract:

Determination of microscopic interactions which give rise to magnetic order in a crystallographic material is a common use of the neutron scattering instruments at the NIST Center for Neutron Research. This is achieved by scattering the neutrons across different vectors of the crystal. However, this does not uniquely determine these spin interactions. Inelastic neutron scattering in which the neutron either imparts or receives energy from the crystal results in a measurable spin wave dispersion at the given vector. Traditionally, researchers would measure as many points as possible; after which they would fit the data against various models to determine the parameters describing the interactions. Much of the data generated using this approach is not necessary to determine the best model. Additionally, the traditional way to determine best fit for a model can lead to many unnecessary parameters being added to arbitrarily make the fit better without being more accurate. We have applied Deep Reinforcement Learning algorithms to simulated experimental data in order to test efficacy of the approach to selection of optimal points to measure for use in determining interaction parameters during experimentation. Deep Reinforcement Learning uses a reward-based system to allow the algorithm to develop a heuristic to achieve the highest reward. So, by rewarding based on distinguishing between models and fitting to the generated experimental data as well as penalizing for taking too many measurements, we are able to train the heuristic to optimize this problem. We have trained the algorithm to select a minimum amount of measurements which will allow for differentiation between two types of simple magnetic models. If successful, this can be applied to more complicated models during experimental planning, cutting down the use of valuable neutron beam time.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Patrick Park		
Academic Institution:	Reed College	**Major:**	Physics
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Find graduate programs with interdisciplinary study of nuclear science and policy		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Reactor Operations and Engineering Group		
NIST Research Advisor:	Dagistan Sahin, Osman Celikten, Joy Shen		
Title of Talk:	Nuclear Design and Analysis of the NIST Replacement Reactor		

Abstract:

Since 1967, the National Bureau of Standards Reactor (NBSR) has produced neutron beams for physics and materials science studies. These beams can determine exact atomic structures, precise material composition of samples, or even create useful medical radioisotopes.

In a 6-month window in 2019, the NBSR received 451 experiment proposals with 2.5 times more days of beam time requested than available. After 54 years of service, the NBSR also has less capacity and more maintenance than newer models overseas. So, many domestic and foreign researchers are seeking nuclear science capabilities outside the United States, such as in France or China.

NIST is thus designing the Replacement Reactor Core, which will be the first U.S. high-performance research reactor of the 21st century. The RRC will have the latest fuels, higher beam powers, and less maintenance than the NBSR. It is cooperatively designed between engineers that design the physical model and scientists that examine the nuclear behavior of that model. Calculating these nuclear parameters involve using Monte Carlo algorithms to predict nuclear reactions via Python and Fortran codes, which can take days to complete on dedicated computational servers.

Specifically, I performed the calculations and analysis of the reactor reactivity as its heavy water is dumped and when its light water moderator or uranium fuel is heated up, which are important nuclear behaviors. Other nuclear properties, like control blade worths and core shutdown margins, were also calculated. These analyses show the RRC is within safe and desired performance margins, which will referenced for engineering design and regulatory compliance.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Ryan Puthumana		
Academic Institution:	University of Maryland, College Park	**Major:**	Bioengineering
Academic Standing (Sept. 2021):	Junior in college		
Future Plans (School/Career):	Currently on pre-med track with future plans in medicine or biomedical research/industry		
NIST Laboratory, Division, and Group:	NIST Center for Neutron Research, Neutron Condensed Matter Science Group		
NIST Research Advisor:	Dr. David Hoogerheide and Dr. Frank Heinrich		
Title of Talk:	Investigating Lipid Bilayer Structures with Neutron Reflectometry		

Abstract:

Biological neutron reflectometry is a powerful scientific technique used to elucidate the structure of nanoscale structures composed of biological materials such as lipid bilayer membranes and membrane-associated proteins. Neutrons are reflected off the sample of interest, and the reflectivity of the neutrons is measured as the ratio of the number of neutrons that reflect from the sample to the total number of incident neutrons. The reflectivity pattern as a function of the neutron momentum transfer, Q, arises from a real space neutron scattering length density (nSLD) profile that encodes the interfacial structural information. Composition space modeling is utilized to derive such a scattering length density profile from the molecular components of the biological interface such as the lipid bilayer headgroups, acyl chains, and solid substrate. Currently, the existing implementations of composition-space modeling for biological neutron reflectometry by the NIST Center for Neutron Research (NCNR) are outdated. They were written in C++, which while fast and effective does not offer the flexibility of a higher-level language such as Python. Python allows for easier integration of the software with instrumental control software and is compatible with modern data-driven experimentation. In my talk, I will describe how I transcribed the existing C++ neutron reflectivity models into Python for various bilayer architectures and produced the “molgroups” module for biological neutron reflectometry data analysis. In addition, I will demonstrate the advanced user-friendliness of neutron reflectivity analysis by incorporating the molgroups module into shareable Jupyter notebooks. These allow a user to run, analyze, and plot existing reflectometry data in a unified workflow.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Jack Rooks

Academic Institution: SUNY at Buffalo

Major: Chemical Engineering

Academic Standing (Sept. 2021): Undergraduate student at SUNY at Buffalo

Future Plans (School/Career): Graduate school

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

NIST Research Advisor: Peter Gilbert

Title of Talk: Assessing Particle Orientation in Small Angle Neutron Scattering

Abstract:

Many materials derive their mechanical strength and flexibility from molecular and nanostructure orientation. The role of orientation is particularly important in materials like plastics, where product performance can rely almost entirely on molecular alignment to confer desired mechanical properties. Thus, measurement and analysis techniques that reveal molecular orientation are vital to optimizing product design and performance. Small angle neutron scattering (SANS) is one such technique that can investigate the nano-scale material structure. Because 2D scattering patterns from SANS are needed to determine particle orientation, data analysis can be challenging. One approach to 2D analysis is through calculation of a parameter called the 'alignment factor' that qualitatively describes how aligned particles are. Several methods have been proposed for calculating alignment factor, all of which are not equivalent. This makes it difficult to compare historical data. Additionally, there is no standard approach when selecting appropriate 2D scattering data for calculation. Here, theoretical alignment factor calculations from simulated 2D scattering patterns for oriented cylinders are used to compare the methods of calculating alignment factor. These theoretical results are supported by experimental SANS data for worm-like micelles. We find the practical limits of each alignment factor method and determine its effectiveness for describing orientation. We propose standards for alignment factor analysis and provide guidelines for selecting suitable data from 2D scattering patterns.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Daven Shah

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

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Graduate School

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

NIST Research Advisor: Caitlyn Wolf, Kathleen Weigandt

Title of Talk: Characterization of Spherical Nanoparticles using Small-Angle X-ray Scattering as a Validation Metric for Neutron Interferometry

Abstract:

Small-angle scattering is a useful technique for characterizing structures at length scales between one nanometer to one micrometer in a range of materials, including nanoparticles, micelles, proteins, and polymers. Small-angle scattering can only provide a sample-averaged picture of the nanoscale structure and lacks spatial resolution, making the study of heterogeneous materials difficult. However, ongoing work in far-field interferometry can enable the collection of spatially-resolved structural information at the same length scales as small-angle scattering. This interferometry data can also be directly related to small-angle scattering data through a Hankel transformation, allowing us to use small-angle X-ray scattering (SAXS) or small-angle neutron scattering (SANS) for validation of new analyses. In this work, we have created a library of analyzed SAXS data for a set of Ludox colloidal silica with a range of radii. Ludox was chosen as our first sample set as they provide a well-characterized model system of spherical nanoparticles as a starting place for validation between new interferometry data and small-angle scattering. In this talk, we will discuss our analysis of these samples. We find that a polydisperse spherical form factor fits the Ludox nanoparticles well at lower concentrations, while at higher concentrations, a Hayter-Penfold structure factor captures the interactions between these charged nanoparticles. Furthermore, because polydispersity and structure factor both affect the transformation of the sphere model between small angle scattering space and interferometry space, effective validation of interferometry data relies on a thorough analysis of the corresponding small angle scattering data.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Aurora Zemborain

Academic Institution: University of Chicago **Major:** Molecular Engineering

Academic Standing (Sept. 2021): 3rd Year

Future Plans (School/Career): Pursue PhD in materials science area with environmental application

NIST Laboratory, Division, and Group: NCNR, NCMS, 6102

NIST Research Advisor: Yuyin Xi, Yun Liu

Title of Talk: Temperature-dependent binary solvent structure of solvent segregation driven gel (SeedGel)

Abstract:

A solvent segregation driven gel (SeedGel) is a thermo-reversible colloidal gel, which forms bicontinuous channels through solvent phase separation induced by temperature change. Unlike bicontinuous interfacially jammed emulsion gel (Bijel) which has its particles jammed at the interphase between the two solvents in the gel phase, SeedGel has its silica particles jammed into one of the solvent domains in gel phase. SeedGel exists in liquid state at lower temperatures and transitions into gel phase at higher temperatures. The project focuses on the scattering data analysis to understand the effects of varying solvent concentrations and temperature on the gel structure.

Wide-angle X-ray scattering (WAXS), small-angle X-ray scattering (SAXS), small angle neutron scattering (SANS), and ultra-small angle neutron scattering (USANS) are all techniques that were used to probe the structures of SeedGel and binary solvents over a wide range of length scales. Scattering experiments were conducted on SeedGel prepared with two binary solvent systems, water/2,6-Lutidine and water/3-MethylPyridine (3MP). Highly charged silica particles with a radius of 13.6 nm were used in both systems.

SeedGel prepared with water/2,6-Lutidine showed a transition point of 26˚C. Structure factors were extrapolated as a function of temperature, which showed a sharp transition around the gelation point at different length scales. A change in contrast is also observed at different temperatures, which is attributed to the solvent exchange between domains.

SeedGel prepared with 3MP exhibited a higher gel transition temperature of 46 ˚C. The data shows that the binary solvent forms nano-sized droplets and their molecules are spaced by a certain repeating distance. Both the nanostructures and the intermolecular distances are highly dependent on the temperature and solvent composition. The temperature-dependent multi-length structures of the solvents are correlated to the phase diagram of the solvents and the properties of SeedGel.

Physical Measurement Laboratory (PML) Participants

William Barrett

Henry Bell

Matthew Belzer

Daniel Bordwin

Emily Buchanan

Joseph Cavanagh

Sadie Chafin

Dillion Cottrill

Jayden Craft

Matthew Diaz

Nicholas Entin

Nora Fayyazuddin Ljungberg

Samuel Felsenfeld

Max Hanrahan

Jason Hsu

Richard Jinschek

Molly Kreider

Physical Measurement Laboratory (PML) Participants (continued)

Hoyean Le

Alexander Loane

John Lundstrom

Satvik Manjigani

Ricardo Morales-Sanchez

Nikita Podobedov

Milan Richardson

Jacob Riddles

Alessandro Rizzoni

Jared Schwartz

Christopher Sherald

Myles Sherman

Catherine Silver

Katherine Slattery

Ross Snyder

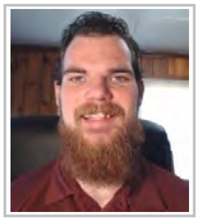
Cassie Stoffer

Ethan Swagel

James Vouzikas

Kendall Zammit

Laura Zhou



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

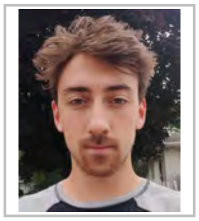
Name: William Barrett		
Academic Institution: Virginia Tech		**Major:** Nanoscience
Academic Standing (Sept. 2021):	Graduated	
Future Plans (School/Career):	Graduate school for nanotechnology and engineering	
NIST Laboratory, Division, and Group:	PML, Microsystems and Nanotechnology, photonics and plasmonics	
NIST Research Advisor:	Amit Agrawal and Henri Lezec	
Title of Talk:	Modulating the Optical Response of Multi-Resonant Nanostructures using Phase Change Materials	

Abstract:

Phase change materials (PCM) have a rich history in computer information storage. Specifically, alloys that come from constituent elements: Ge, Sb, Te. The alloy Ge2Sb2Te5 (GST) can undergo electrical or optical pulse melt-quenching, and switch between amorphous and crystalline states on a nanosecond timescale. These phases also have large differences in refractive index and resistance which make them promising candidates for non-volatile memory or rewritable optical storage. Using this mechanism of active modulation of PCM properties, one can modulate spectral resonances of subwavelength photonic devices and achieve higher optical contrast as it is switched between phases. Achieving a device that can bridge the two ideas of optical and electrical memory storage may be achievable via combination of a PCM and multi-resonant nanophotonic structures.

Two device embodiments were studied using the finite-difference-time-domain technique to model their electromagnetic response. The first, metal-insulator-metal nanopillar array that utilizes surface plasmon polaritons (SPPs) to achieve a multi-resonant optical response. The second, a Huygens' metasurface that leverages Bound states in the Continuum to achieve high-quality factor resonant response. Using GST, one can actively modulate the optical responses of these devices by altering the phase of GST which can disrupt the underlying mechanisms governing the spectral resonances, and achieve high contrast switching.

By performing full electromagnetic simulations by varying the phases of GST in these two device geometries, their transmission and reflection were collected and analyzed. The result show complete disruption of SPP generation between the GST and metal in the nanopillars device in one of the phases. For the Huygens' metasurface, preliminary simulations suggest that the GST switching will significantly improve the spectral modulation depth of the high-quality factor peaks.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Henry Bell

Academic Institution: Macalester College

Major: Physics, Mathematics

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Graduate School

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Nanoscale Device and Characterization Division, Advanced Electronics Group

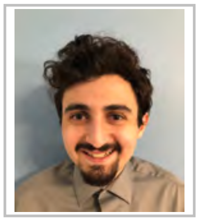
NIST Research Advisor: Dr. Sujitra Pookpanratana

Title of Talk: Custom Calibration and Correction of Photoemission Electron Microscope Images

Abstract:

In 2019, a photoemission electron microscope (PEEM) was delivered and installed on the NIST Gaithersburg campus. The PEEM is a full-field electron microscope that utilizes the photoelectric effect to image a surface. It is a useful tool because it has resolution on the scale of 10 nanometers and can image both the morphology of a surface and its electronic properties. These two imaging techniques can be applied to further understand the electronic traits of materials for use in electronic devices, for example.

While the hardware of the PEEM was built commercially, the calibration and processing procedures had to be developed in-house. The real space images produced by the PEEM can, in most cases, be manually corrected with small datasets. These corrections include bright field, dark field and thermal drift corrections. For momentum space images, rotations, pixel calibrations, and energy alignment calibrations must be completed. These operations are difficult to complete manually with existing software. I have developed custom Python scripts to both automate this process and standardize the calibration and correction procedure to streamline data analysis for users of the PEEM. Graphene was utilized as an initial calibration material due to its distinct electronic band structure. The 6 Dirac cones of graphene were used as iso-energy points to align the frames on the energy-axis and a series of matrix operations were utilized to rotate the image in the momentum axis to correct for sample misalignment.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Matthew Belzer		
Academic Institution:	Stony Brook University	**Major:**	Physics and Applied Math
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Graduate school to get my PhD in physics		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science Division, Optical Radiation Group		
NIST Research Advisor:	Dr. Maritoni Litorja		
Title of Talk:	Assembly of Remote-Controlled Miniature LED Assembly		

Abstract:

Currently, most detectors used for biology research that measure light in the femto to nanowatt ranges are not SI traceable. Instead, these detectors use proprietary units called Relative Light Units. Therefore, it is difficult to properly calibrate these detectors since it is unknown what the actual light emission should be. Additionally, the lack of calibrated light sources prevents scientists from measuring the light emission, in SI units, of certain chemical processes, like the production of oxyluciferin, the familiar firefly glow, which is used as a chemical tag for a variety of biological measurements. To calibrate these detectors using SI units, I had to design and build an LED light source that emits a steady amount of light at certain wavelengths. Since the current relates to the light emission of an LED, I have to limit the current to the nanoamp range using a gigaohm resistor. Another important design requirement is remote control, since physically pressing the device on and off could cause slight shifts in its location, changing the amount of light received by the detector. A cost effective way to achieve this is to use the Arduino Wifi REV2 device, since it is easily programmable and can receive commands over Wifi. The final consideration is having an extended light source instead of a discrete source because it makes it easier to precisely measure the light. Organic LEDs (OLEDs) are extended light sources because they are built by placing an organic semiconductor layer between two electrodes. These layers are larger than the semiconductor chips that typical LEDs use. OLEDs have recently become commercially available for display technologies, making them cost effective as well. As such my design for the light source will consist of an Arduino controlling an OLED display that has a nanoamp current running through it.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Daniel Bordwin

Academic Institution: University of Maryland

Major: Physics and Astronomy

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Obtaining bachelor's degree and seeking employment in industry.

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

NIST Research Advisor: Dr. Jon Geist

Title of Talk: Assessing the causes of uncertainties within triaxial accelerometers

Abstract:

Accelerometers are used in a wide array of devices in a wide array of industries. With their ubiquitous nature, it is important to know what will affect the outputs they give. These uncertainties are important to study and understand, with their causes needing to be properly identified. The simulations presented are carried out by rotating the apparatus containing the accelerometers in the local gravitational field from multiple starting orientations. From this, the response of the accelerometers are assumed to take a linear form with an intrinsic set of offsets added to the product of a sensitivity matrix and the acceleration felt by the device. Sample sensitivity matrices and offset triples are then generated and inputted in order to create the full dataset. The assumption from here is that the data will take the form of a summation of a sine and cosine with coefficients along with a constant. The data generated is then fitted in this form in order to find intrinsic properties involving the sensitivity matrix, offsets, and dot products between the axes of maximum sensitivity of the three accelerometers. The uncertainties in the intrinsic properties and sensitivity matrices were not found to be caused by the accelerometers being non-orthogonal. Rather, it was found that the significant uncertainties in the intrinsic properties of the triaxial accelerometer are due to improper installation and construction. This is important because it shows manufacturers and customers what should be focused on the most. While there should still be efforts to keep the non-orthogonality as small as possible, most of the focus should be on the precise installation and construction of the devices.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

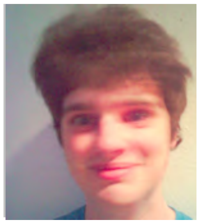
Name:	Emily Boone Buchanan		
Academic Institution:	The University of Texas at Dallas	**Major:**	Chemistry and Biology
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Graduate School		
NIST Laboratory, Division, and Group:	Physical Measurements Laboratory, Applied Physics Division 686, Magnetic Imaging Group		
NIST Research Advisor:	Stephen Russek, PhD		
Title of Talk:	Utilization of Hyperpolarization in the Development of a Micro-MRI Imaging System		

Abstract:

Magnetic Resonance Imaging (MRI) is a standard radiation-free medical technique which uses strong magnetic fields to image water protons in the body and generate anatomical images. In addition, specialized pulse sequences can be used in MRI studies to discern specific information about the local chemical environment (T1, T2, Diffusion) which is used to identify and diagnose certain diseases and cancers. Current micro-MRI systems use large superconducting magnets to image tissues with best resolution near 20 um. However, these systems still cannot resolve cells or cellular structures. Improved resolution and contrast are highly desirable for in vitro imaging of cell lines and tissue biopsies. In addition, small, more compact systems are required for use in pathology and personalized medicine applications to analyze the response of patient derived cell cultures to different therapies over time.

The goal of this project was to develop a portable, cryogen free, low cost microMRI system for cellular imaging. To overcome the inherit signal to noise challenges and long scan times required in conventional MRI our system is perfused with hyperpolarized water generated by a novel integrated solid-state hyperpolarizer which operates at low field and room temperature. Concurrently, we developed a protocol to fabricate liposomes loaded with an MRI contrast agent with dimensions ranging from 100 nm to 5 um to serve as cell mimics and reference standards for cellular imaging below the current 20 um limit.

A spin echo multi-slice pulse sequence was optimized on a conventional superconducting microMRI operating at 3T and an imaging resolution of 30 um was obtained. The imaging protocols were then transferred to a smaller hyperpolarized microMRI system operating at 135 mT, which was built in house by the Magnetic Imaging Group. The imaging pulse sequences were extended to control the hyperpolarizer and sample bias, allowing the study of hyperpolarization as a function of microwave frequency and power, as well as hyperpolarizer-sample electrochemistry.



SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name: Joseph Cavanagh

Academic Institution: Brown University	**Major:** Chemical Physics

Academic Standing (Sept. 2021): Senior

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

NIST Laboratory, Division, and Group: Boulder, PML, Quantum Nanophotonics

NIST Research Advisor: Krister Shalm

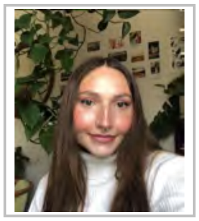
Title of Talk: The Ultimate Coin Flipper

Abstract:

Random numbers are ubiquitous tools in today’s world of computing, used in everything from auditing election ballots to video games to encryption. The best widely used random number generators (RNGs) turn environmental noise into a source of randomness. However, there’s no way to bound the entropy, or “how random” the RNG’s outputs are for these, without an inordinate number of samples. Even if one extensively tests hardware RNGs, new biases might appear over time, well after testing. However, recent experiments at NIST have created a RNG without these difficulties, using the laws of quantum physics.

Quantum systems can exhibit a phenomenon called entanglement, leading to correlations between observations that can be explained by either faster-than-light signaling or true randomness. As long as we assume that it isn’t possible to send information faster than the speed of light (a very good assumption, otherwise many other physical theories would need to be rewritten), we can create an unpredictable sequence of bits by making measurements on entangled systems. A mathematical result then quantifies the entropy of those bits. Finally, we can “extract” that entropy to construct a random number with a known bias, eliminating the need for testing large samples.

Using entanglement, NIST is working on satisfying the public demand for random numbers by adding this source of certifiable randomness to its “randomness beacon” broadcasting 512 random bits every minute. Unfortunately, the is quite slow. The previous run took months, with a significant portion of that time dedicated to the data processing, using a series of different programs with different authors and dependencies. My current work focuses on turning months of work into minutes, by automating all of the data processing. This talk will elaborate on the inner workings of and my role in automating this new source of randomness.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Sadie Chafin

Academic Institution: West Virginia University **Major:** Physics

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Work in Industry or National Lab

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

NIST Research Advisor: Andrew Madison

Title of Talk: Automation of a hyperspectral confocal laser scanning microscope

Abstract:

Confocal laser scanning microscopy is a mainstay of modern metrology, enabling sensitive measurements of photoluminescent samples with both high specificity and high spatial resolution. Such measurements directly impact ongoing research efforts as diverse as the nanofabrication of quantum emitters and the chemical analysis nanoplastics. In traditional confocal microscopes, optical filters coarsely divide continuous emission spectra into discrete bands that reduce specificity of the measurement and are subject to spectral crosstalk in the presence of heterogeneous emitters. This problem of spectral ambiguity degrades the performance of the microscope, at best, and corrupts the reduction of image data, at worst. To solve this problem, we are integrating and automating a spectrograph into a custom confocal laser scanning microscope to spectrally resolve optical responses of disparate samples including gallium arsenide quantum dots, fluorescent polystyrene nanoparticles, and polymeric nanoplastic arrays. Automation of our new microscope is central to this stage of the project. In addition to developing hardware drivers that control laser scanning, widefield illumination, inspection imaging, and stage positioning, we are developing a graphical user interface that facilitates rapid system configuration and data collection. This presentation will report on progress of the integration and automation of key subsystems of a hyperspectral confocal laser scanning microscope.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Dillion Cottrill

Academic Institution: West Virginia University **Major:** Physics/Economics

Academic Standing (Sept. 2021): First year graduate student at Stony Brook University

Future Plans (School/Career): Study Quantum Information/Quantum Computing

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Microsystems and Nanotechnology Division, Nanostructure and Fabrication Group

NIST Research Advisor: Dr. Marcelo Davanco

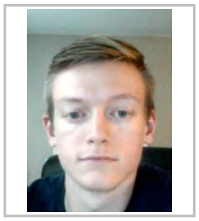
Title of Talk: AlGaAs metalens for on-chip waveguide single-photon sources

Abstract:

Electromagnetic radiation from point dipole light sources is difficult to manipulate with conventional free-space optics. Metasurfaces are geometries with subwavelength features that can be engineered to allow free and effective control of the wavefront of light beams, allowing radical manipulation of the flow of light. Epitaxial quantum dots are nanoscale semiconductor heterostructures embedded in semiconductor wafers which act as dipole emitters, producing single photons. Metasurfaces allow for directed confinement of these photons, which may be funneled into an on-chip waveguide with high efficiency.

Using a finite difference time-domain simulation software, we have designed a planar metasurface to perform this task. Using a simple equation describing phase shift as a function of position, we have designed a metalens for in-plane phase manipulation to more effectively couple light into a photonic waveguide.

After simulation is complete, the metasurface will be constructed on our own device. Our geometry is an alternative to existing methods for collecting photons in epitaxial quantum dots. Our design is non-resonant, which allows efficient collection of emission over a broad wavelength range without the need for spectral tuning the quantum dot. This design also avoids extreme proximity of the quantum dot to etched sidewalls, which causes decoherence of emitted photons.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Jayden D. Craft

Academic Institution: Stockton University

Major: Applied Physics/Applied Mathematics

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): I plan to go to graduate school to obtain a PhD in Physics after which I plan to work in industry.

NIST Laboratory, Division, and Group: PML, Nanoscale Device Characterization Division, Nanoscale Processes and Measurements Group

NIST Research Advisor: Robert McMichael

Title of Talk: Sequential Bayesian Experiment Design

Abstract:

In this talk we focus on sequential Bayesian experimental design, an adaptive method that makes measurements faster and more efficient. In sequential Bayesian experimental design, we adaptively choose new, optimal, settings for experiments while accounting for measurement noise. From the measurement noise properties, we can find the probability that our possible parameter values are true to our system with the most likely values selected as the "true" values for that iteration. Like curve fitting in excel, we want to find the best model for our data which means we need the best possible parameters (coefficients if it were a polynomial). Our method then estimates the utility (cost) of different measurement settings and picks high-utility settings for the next measurement. Then we make a new measurement with our improved settings which will give us a more informed model using the most probabilistic parameters and give even better settings. The decisions that are made about our settings in each step of this sequential process rely on predicted changes in information entropy, which is not always simple to compute. Currently we use a crude, mostly effective, estimate using the variance of our samples, so we are currently exploring new, computationally efficient, ways to calculate the information entropy. We have some ideas as to why our crude method does not always work, but true entropy will always work, which is why finding efficient ways to calculate entropy is important. However, with the current crude estimate of entropy, sequential Bayesian experiment design works very well, focusing measurements on the most sensitive settings while avoiding uninformative settings. We find that the sequential Bayesian experimental design method converges to accurate parameter values faster than other experimental automation methods. Overall, our software performs better than traditional experiment automation, which means we are that much closer to having computers that not only interpret data, but also guide data collection. Current software at https://github.com/usnistgov/optbayesexpt.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Matthew Diaz

Academic Institution: University of Maryland

Major: Physics

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Graduate school: PHD program

NIST Laboratory, Division, and Group: PML, 682.03, Neutron Physics Group-Radiation Physics Division

NIST Research Advisor: Elizabeth Scott

Title of Talk: Simulating Charged Particle Energy Deposition

Abstract:

Neutron beta decay is the process where a neutron decays into a proton, electron, and antineutrino. The primary goal of the project is to use a cryogenic superconducting detector for energy measurement of charged particles of neutron beta decay. A superconductor below a critical temperature has zero resistance but some finite impedance, which in combination with a resistor allows for the construction of a resonant circuit. As temperature is added to the superconductor due to it being struck by charged particles, the impedance of the superconductor and by extension the circuit is altered. The project measures the change of the circuit's resonant frequency, which is dependent on the circuit's impedance, by passing an AC current through the circuit. Therefore, the energy deposited can be measured by analyzing the resonant frequency change of the circuit. This summer I worked on using Geant4, a Monte Carlo toolkit that allows for simulations of particles in matter, to create an in-depth simulation for energy deposition and thermal transport in the detector. The simulations' goal is to model an incoming electron striking a detector, and the heat propagation from the electron strike. This is possible using the G4CMP Geant4 extension package which allows modeling of phonon physics within silicon. Phonons are a measurement of the heat, or kinetic energy, in a crystal lattice. By having the electrons hit a crystal lattice of silicon we could see how the heat was being dispersed through the detector by tracking the phonons that were created, which allows a better fine tuning of the detector design.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name:	Nicholas Entin		
Academic Institution:	University of Colorado Boulder	**Major:**	Physics, Mathematics
Academic Standing (Sept. 2021):	Junior		
Future Plans (School/Career):	Graduate school, then academic research, government research, or private industry.		
NIST Laboratory, Division, and Group:	Boulder, PML, Quantum Nanophotonics		
NIST Research Advisor:	Dr. Sae Woo Nam		
Title of Talk:	Developing Open-Source Hardware for Superconducting Single-Photon Detectors		

Abstract:

Superconducting nanowire single-photon detectors (SNSPDs) are powerful measurement devices that are able to detect the smallest unit of light. They are being used in many experimental setups that require high spatial and temporal resolution. However, no standardized electronics exist for processing the signal from the detectors so that it can be recorded by a computer. This project seeks to design simplified open-source hardware for processing these signals. When a photon hits the nanowire, a small current pulse is created, which is amplified and converted to a voltage pulse. A comparator circuit is used to convert the small voltage pulse into a digital logic level that can be recorded by a computer. This circuit requires a threshold voltage input to compare to the voltage pulse. In the new hardware design, a microcontroller connected to a USB port is used to power and control the comparator circuit. In order to create a threshold voltage for the comparator, a digital output of the microcontroller board is used to generate a pulse-width modulated signal (PWM) that is converted to an analog voltage level with a low-pass filter, creating a digital-to-analog converter (DAC). Different low-pass filter designs were explored to understand the quality of the analog voltage level. In addition, the comparator circuit and PWM DAC were tested using simulated voltage pulses that replicate those from a detector. In this talk, I will describe the SNPSD device and my progress in the development of open-source hardware for SNSPDs. The results of this project will contribute to these high-efficiency detectors being easier to use in many different applications.

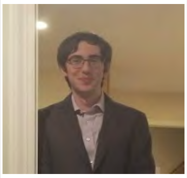
SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name:	Nora Fayyazuddin Ljungberg		
Academic Institution:	Wellesley College	**Major:**	Physics, mathematics
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	PhD in physics		
NIST Laboratory, Division, and Group:	Boulder, Physical measurement laboratory, applied physics division, quantum nanophotonics		
NIST Research Advisor:	Krister Shalm		
Title of Talk:	Optimizing detection probabilities of entangled photons		

Abstract:

Quantum entanglement is an idea that is necessary for an understanding of quantum mechanical processes as well as advancements in quantum computing. It describes the fact that two quantum states can be connected to each other even when the particles described by these states are spatially far apart. Spontaneous parametric downconversion (SPDC) is one of the most common methods of producing entangled photons. In this process, one photon, called the pump, is sent through a specially optimized crystal where it spontaneously splits into two entangled photons, called the signal and the idler. In my time at NIST, I have been working with a group that models the process of downconversion in order to calculate various quantities relevant to the process. They have created a web-based tool and a Python library of functions that simplify some of the calculations to model downconversion. One of the quantities that the library calculates is heralding efficiency, which is the likelihood that one of the photons will be detected in a particular spatial mode given that the other has already been detected in that mode. A high heralding efficiency is vital to creating usable photonic quantum bits for computations. One of my roles has been to compare the results of this library to established approximations. In my talk, I will discuss the importance of downconversion and heralding to quantum applications, as well as my own role in checking the results of the library.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Samuel Felsenfeld

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

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): Either some kind of engineering industry job or graduate school.

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

NIST Research Advisor: Dr. Joseph Tan

Title of Talk: Charged particle dynamics in a 0.7 T Unitary Penning Trap / Electron Beam Ion Trap

Abstract:

Ion trapping has many applications, ranging from precision measurements of fundamental constants to the creation of atomic clocks to measure time. Traps requiring strong static magnetic fields like Penning traps and electron beam ion traps (EBITs) are often expensive to maintain since they require a constant power supply and cooling to sustain their powerful electromagnets. As an alternative to traps that require electromagnets, we studied compact permanent magnet ion traps for the production and capture of highly charged ions. The two systems we simulated were a cylindrical Penning trap and an electron beam ion trap, each using a similar configuration of electrodes and Halbach arrays of permanent magnets to create a magnetic field of ~0.75 T at the trap center, with adjustable electrical potential well depth. A Penning trap is an ion trap designed to confine a charged particle in a small volume using a magnetic field and electrostatic potential well to make it oscillate in a controlled fashion. An EBIT is similar but includes an intense electron beam aligned with the trap axis and square-well electrostatic potential, enabling it to further ionize atoms in the trap as well as provide tighter radial confinement. In this work, through simulations using the Lorentz software, we found that the new 0.75 T Penning trap would readily confine Pr X (9 times ionized), Kr XVII, Ar XIV, and bare Ne at an initial energy of 5 eV; moreover, the motion of these ions trapped at much lower energies (less than 0.5 eV) agreed closely with the theory for idealized Penning traps with hyperbolic electrodes. We analyzed these deviations from theory to evaluate the effects caused by ions not being tightly confined axially to the trap center. For the electron beam ion trap, we created a program to quantify the current density and energy of the beam as a function of position in the trap. Although the electrode potentials can be readily optimized for an electron beam that neglects self-repulsion, we are working to determine the maximum beam current that the mini-EBIT can support at various energies if Coulomb interaction (space charge) in a realistic electron beam is accounted for.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Max Hanrahan			
Academic Institution:	Hamilton College	**Major:**	Physics
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Career in applied math or physics, or continuing my physics education in graduate school.		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurements Division, Mass and Force Group		
NIST Research Advisor:	Michael Gaitan		
Title of Talk:	Calibration of Three-Axis Accelerometer and Gyroscope Using Pendulum-Based Excitation		

Abstract:

Accelerometers are devices capable of sensing acceleration. They are used in machines such as vehicles, cellular phones, and video game sensors. They are especially important in vehicles when GPS services are not available. We developed a method to calibrate a 3-axis accelerometer and gyroscope under dynamic conditions, using pendulum excitation. The device under testing is a battery-operated Arduino microelectromechanical system (MEMS) capable of transmitting its readings to a computer via Bluetooth. Our intrinsic properties model is based on the assumption that the device may have some intrinsic offset. We account for this by first calibrating the device in static conditions. To do so, a cube was built to measure the accelerational intrinsic sensitivity and offset along for each of the three accelerometers. These measured sensitivity and offset values that are then used in the rotational calibration. A pendulum was built to excite the accelerometers and gyroscopes to calibrate the rotational sensitivity of the gyroscope under dynamic conditions. A calibration analysis was then performed by fitting the measured acceleration and rotation data to an equation for pendulum motion. Uncertainty was determined from the covariance of the parameters in the fit. We compare the results of our calibration to the manufacturer's advertised sensitivities and uncertainties, and assess the effectiveness of our pendulum-based calibration method.

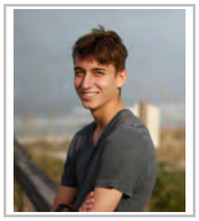
	**SURF Student Colloquium** NIST – Gaithersburg, MD August 2-6, 2021

Name: Jason Hsu

Academic Institution:	University of Maryland, College Park	**Major:**	Electrical Engineering
Academic Standing (Sept. 2021):	Sophomore		
Future Plans (School/Career):	Graduate Degree		
NIST Laboratory, Division, and Group:	Physical Measurement Labratory, Biophysical and Biomedical Measurement Group		
NIST Research Advisor:	Dr. Gregory Cooksey		
Title of Talk:	Automated Collection and Control of Flow Cytometry on a Microchip		

Abstract:

Flow cytometry has become an important tool in various fields, due to its capacity to process and measure multiple simultaneous optical signals from thousands of individual objects (typically cells) per second. An instrument collects data for each object that indicates parameters such as cell size, granularity, and various aspects of cell type or activity (as indicated by emission of fluorescent biomarkers that indicate the abundance of target molecules). For commercial cytometers, automated analysis is standard, although the signals are simplified to scalars such as total integrated intensity. These data, along with limited information about system configuration, make it very challenging to find rare events such as circulating tumor cells in a sample. We are developing a system that improves counting accuracy and signal uncertainty using precise control of flow and modulation and collection of light through multiple optical paths. Our system requires integration and automation of additional components, which is being built through a central MATLAB graphical user interface. First, there are signal generators that modulate several lasers, each of which excites cells in different parts of the system. Light from each region is then guided to a power supplied photodetector where it is converted to an electrical signal that is then amplified and digitized. My project has specifically focused on control and readout from each component, such that we can reach the project goal of continuous collection and processing of 16-bit digitization at gigabyte per second in real time. Commands for each device were adapted to interface with MATLAB using serial object commands and memory mapping from C to MATLAB. This project will streamline the tasks of data collection and processing, and allow better statistics for the detection and characterization of rare objects in flow cytometry.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Richard Jinschek		
Academic Institution:	Lake Forest College	**Major:**	Physics & Computer Science
Academic Standing (Sept. 2021):	Third Year Undergraduate		
Future Plans (School/Career):	Graduate School / Law School, work in Patent Law.		
NIST Laboratory, Division, and Group:	Physical Measurements Lab, Quantum Measurement Division, Applied Electrical Metrology Group		
NIST Research Advisor:	Dr. Richard Steiner		
Title of Talk:	Characterization of Fluke 8588 Reference Multimeter to Digitize and Analyze Power Data		

Abstract:

The Fluke meter 8588A is a relatively new Reference Multimeter claimed to be very stable in comparison to other digitizing multimeters and is advertised as being designed for calibration and use in metrology laboratories. The meter released in early 2019 features multiple measurement functions, of which 2 will be investigated in this project, the digitized DC current (DCI) and digitized DC voltage (DCV) functions. The focus of this project is to test the Fluke meter under different conditions in order to find corrections that can be used at high sampling rates in the DCI and DCV modes. Especially of interest for the DCI and DCV functions is how their accuracy is affected by varying other parameters such as the signal frequency, number of periods, and pts/period. The nonlinear behavior of the results will be adjusted with correctional factors to make the measurements more linear. The long-term goal of the project is to use the Fluke Reference Multimeter to digitize and analyze AC power data. Additionally, similar characterization was done on a simpler sensor plus digitizing system for NetZero House power data.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name: Molly Kate Kreider

Academic Institution: University of Richmond **Major:** Physics

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Attend graduate school & pursue a career in research

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Time and Frequency Division, Optical Frequency Measurements Group

NIST Research Advisor: Scott Diddams

Title of Talk: Modeling mode shifts in astro-etalons for high precision spectrographic calibration

Abstract:

Fabry-Pérot (FP) etalons, optical cavities formed by two parallel mirrors, are used for spectrographic calibration in a wide variety of applications. An FP etalon takes broadband, continuous input light and outputs a spectrum of discrete wavelengths called modes, and this well-defined, comb-like spectral output makes etalons well suited for application in radial velocity (RV) exoplanet detection. However, RV measurements can require fractional precision on the order of 10^-9, making careful study of etalon systems and their mode stability critical. Recent studies of several etalon systems indicate that over time, an etalon's modes experience a complex chromatic-dependent drift, and understanding the mechanism behind this drift is necessary to design etalons that can achieve higher RV precision. In this work, we employ Fresnel analysis and the transfer matrix method to model the phase shift of light in the etalon system to study possible sources of this behavior, including changes to the mirror coatings caused by small temperature changes (~1 mK) in the system and small variations in incident angle of light on the cavity. We study the individual effect of each parameter change on the spectrum and model several combinations of parameter changes meant to test possible physical explanations for the behavior. While parameter variation led to Doppler shifts showing qualitative agreement with earlier measurements of mode shift, exact agreement and conclusive predictions are still not realized. Overall, these results do not therefore provide conclusive evidence of the mechanism behind the chromatic dependence of the mode shifts, but they do both exclude some simple explanations for the measured behavior and, more importantly, provide insight into the sensitivity and stability of FP etalons, which is crucial to further understanding and stabilizing etalon systems for radial velocity measurements.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Hoyean Le		
Academic Institution:	Georgia Institute of Technology	**Major:**	Mechanical Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	PhD in Fluid Mechanics		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science Division, Fluid Metrology Group		
NIST Research Advisor:	Dr. John D. Wright and Dr. Aaron N. Johnson		
Title of Talk:	Simulating the Simulator – A Computational Fluid Dynamic Analysis of NIST’s Stack Simulator		

Abstract:

NIST's Scale-Model Smokestack Simulator (SMSS) is a unique research facility designed to improve the flow measurement accuracy of sensors and methods used to quantify greenhouse gases and other pollutants from smokestacks. With the imminent closure of the SMSS and steady advances of commercial Computational Fluid Dynamics (CFD) programs, this study investigated the feasibility of replacing the SMSS with a virtual smokestack simulator. (CFD programs numerically solve the governing equations of fluid motion – the Navier-Stokes equations – in complex geometries too difficult to solve analytically.) If successful, a CFD-based virtual stack simulator would allow us to inexpensively test various probe and smokestack configurations. We used CFD to calculate velocity profiles in the SMSS and the outputs of multi-path ultrasonic flow meters and compared them to experimental results from the real SMSS.

We numerically simulated the turbulent flow in the SMSS facility using the Reynolds Averaged Navier Stokes and the k-omega turbulence model, which we solved using the commercially available COMSOL Multiphysics software. The model produced 3D velocity profiles in the straight "reference" section of the SMSS as well as the much more challenging "test" section that is downstream of a sharp elbow where large swirl is known to exist in the real facility. Pitch and yaw angles of the swirling flow in the test section were severely underestimated by the model, probably due to artificial diffusion applied in commercial programs to promote convergence of the numerical simulations. Simulated outputs of multi-path ultrasonic flow meters installed in the reference and test sections were compared to actual measurements made in the SMSS. Results suggest that this CFD model is unable to replace the measurements taken by physical sensors but may still be useful in determining the qualitative differences between various possible configurations of smokestacks and ultrasonic meters.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Alexander Loane			
Academic Institution:	Cornell University	**Major:**	Mechanical Engineering
Academic Standing (Sept. 2021):	Graduate Student (Graduated May 2021)		
Future Plans (School/Career):	Master of Engineering at Cornell University		
NIST Laboratory, Division, and Group:	PML, Quantum Measurement Division, Applied Electrical Metrology Group		
NIST Research Advisor:	Dr. Allen Goldstein		
Title of Talk:	Calibration of Smart Grid Simulation Response to Oscillatory Waveforms		

Abstract:

The NIST Smart Grid program aims to advance measurement science that will improve grid efficiency and reliability while enabling greater use of renewable energy sources in the grid. These goals are achieved through research, standardization and testing which require the development of Power Hardware-In-the-Loop (PHIL) capability with a connected Grid Emulation model, Real Time Simulator (RTS), Amplifier, and Battery Simulator to mimic the behavior of electric network with connected renewal energy sources. PHIL systems need to be calibrated and periodically validated in order to ensure fidelity and accuracy of the results they produce.

This project develops a calibration tool for the PHIL capability that is particularly suited to generate PHIL test signals containing multiple frequency components and provide users the ability to perform closed loop stability tests. Further, the calibration tool will use a state space representation for test signals that would permit external modulation of the test signal while also confining the evolution of the test signals to known manifolds within the state space representation. This new technique will be implemented using a Real Time (RT) processor, Field Programmable Gate Array (FPGA) based signal conditioning, laboratory grade digital to analog (DAC) and analog to digital converter (ADC). All these components have to be evaluated and characterized thoroughly in to prove this approach feasible. If shown to meet the desired accuracy and performance requirements, this system will be integrated into the NIST Smart Grid Testbed facility and other PHIL test system used by the Department of Energy to validate grid stability in response to renewable generation.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name:	John Lundstrom		
Academic Institution:	Regis University	**Major:**	Computational Physics and Mathematics
Academic Standing (Sept. 2021):	Alumni		
Future Plans (School/Career):	Work in industry for 1-2 years, then pursue graduate school		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Applied Physics Division, Magnetic Imaging Group		
NIST Research Advisor:	Katy Keenan (PML) and Andrew Dienstfrey (ITL)		
Title of Talk:	Non-Linear Optimization for Enhanced Parameter Retrieval in Magnetic Resonance Fingerprinting		

Abstract:

Quantitative Magnetic Resonance Imaging (qMRI) is emerging as a critical tool in medical diagnostics. However, methods for qMRI demand long scan times to provide high-quality quantitative maps. Magnetic Resonance Fingerprinting (MRF) is a novel method for simultaneous multiparametric quantitative image acquisition, which is five times faster and potentially more accurate than traditional quantitative map methods. The current MRF analysis pipeline uses dictionary matching to infer MR parameters. In this algorithm, one compares under-sampled MRI data to a model-based dictionary of unique MR parameter combinations; the quantitative MRF maps are determined by the closest match. In using dictionary matching, we are constrained to a discrete table of parameter values, whereas in reality, these values are continuous. We add non-linear optimization to this step of the analysis with the goal of obtaining more precise and accurate parameter results than dictionary matching alone. We quantify the errors in both methods, dictionary matching and non-linear optimization, using a Monte Carlo simulation. Estimating uncertainty in parameter values will lead to a better understanding of MRF function and improve its utility in a clinical setting.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Satvik Manjigani

Academic Institution: University of Maryland, College Park

Major: Physics and Astronomy

Academic Standing (Sept. 2021): Sophomore

Future Plans (School/Career): I plan to pursue a PhD 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: Using Machine Learning to Characterize DNA Structures

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 Deep Neural Network to classify DNA structures in a binary model. Using the radius of gyration of simulated DNA strands, we train Machine Learners to classify the strands as either folded or unfolded. 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 2-6, 2021

Name:	Ricardo Morales Sanchez
Academic Institution:	University of Puerto Rico at Humacao
Major:	Physics applied to electronics
Academic Standing (Sept. 2021):	Senior
Future Plans (School/Career):	Attend a PhD program for materials science and engineering.
NIST Laboratory, Division, and Group:	PML
NIST Research Advisor:	Dr. Akobuije Chijioke
Title of Talk:	Resonator modeling for novel sound calibration technique

Abstract:

Calibration is an important task that must be done for sound recording instruments (most commonly laboratory standard microphones) at the National Institute of Standards and Technology (NIST). The need to improve the calibration techniques has led to the discovery of using refractive index as a novel technique for sound calibration. The use of a cylindrical design for a resonator would be ideal to accurately calibrate these sound recording instruments. The resonator will consist of a stainless steel cylinder that will hold a sound generator (piezoelectric) at one end and the sound recording instrument on the other end. On the sides there will be two two-way mirrors that will reflect a beam inside the acoustic field of the cylinder. The presence of the acoustic field will change the refractive index of the air inside the cylinder and will affect the laser beam. The laser beam will indicate how much the acoustic pressure has changed inside the cylinder; giving the necessary information for the engineer to calibrate the sound recording instrument. By using the COMSOL Multiphysics modeling tool, a basic model of the resonator was designed and studied. Based on the different eigenfrequencies studied, a sound field was modeled to observe the behavior of the resonator itself. As the project advances, a different acoustic cavity might prove more useful for different eigenfrequencies and/or different sound measurement instruments.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Nikita Podobedov

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

Academic Standing (Sept. 2021): Graduated

Future Plans (School/Career): Graduate School

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Biophysical and Biomedical Engineering Group

NIST Research Advisor: Dr. Gregory Cooksey

Title of Talk: Graphical User Interface for Analysis of Data from a Serial Microfluidic Cytometer

Abstract:

High throughput measurement of cells is crucial to many key applications in medicine, like drug discovery, cancer screening, and therapeutic monitoring. Such measurements are commonly done using flow cytometers – measurement instruments which have throughputs on the order of tens of thousands of cells per second. In a flow cytometer, cells tagged with fluorescent biomarkers move along a microfluidic channel where they pass through a laser. Emitted light is captured by optical waveguides and recorded by photodetectors. However, each cell is only measured once, and the recorded values are reduced to scalars. This limits the ability to characterize biomarker distributions with high precision, reducing the capacity to discriminate small changes within a population and to distinguish rare objects. To characterize and improve measurement uncertainty, we have developed a novel cytometer which contains multiple measurement regions. Measurements are repeated four times along the flow path and are recorded as high-resolution intensity-over-time signals. This data format necessitates novel analysis software that can process the unique features of our cytometer, like visualization and analysis of the intensity profile and measurement precision for each object. A data analysis graphical user interface (GUI) was developed in MATLAB with those features. This GUI was also utilized to set up comparisons between traditional flow cytometers and our novel device. Serial cytometer data sets were first converted to be interoperable with current data standards for cytometry, and traditional comparison metrics like cytometer sensitivity were built into the GUI. Overall, by reducing measurement uncertainty, the serial cytometer holds promise for improving decision making in fields of medicine where cytometers are used.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Milan Richardson

Academic Institution: University of Maryland Baltimore County (UMBC) **Major:** Bioinformatics and Comp. Biology

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): To obtain an MD/PhD in graduate school.

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

NIST Research Advisor: Dr. Michael P. Zwolak

Title of Talk: Employing Machine Learning to Classify Bimolecular Translocation Events

Abstract:

The ionic current flowing through nanopores enables measuring and distinguishing biomolecules as they translocate through the pore. The change in ionic current as the molecule enters the pore is one characteristic feature that reflects molecule size and type. The duration of the event and waiting time between events also provide characteristics features. The distribution of all these features provides the means to statistically distinguish different molecular events, but it is not the only information present in ionic current time traces. We employ machine learning to classify bimolecular translocation events within experimental data on DNA translocation, as well as synthetic data, to determine what features enable accurate classification.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Jacob Riddles		
Academic Institution:	The University of North Carolina at Charlotte	**Major:**	Mechanical Engineering
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Graduate School, Work in Industry		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Sensor Science Division, Dimensional Metrology Group		
NIST Research Advisor:	Dr. Meghan Shilling		
Title of Talk:	Simulating the Effects of XCT System Geometry Errors		

Abstract:

X-Ray Computed Tomography (XCT) is a nondestructive imaging technique used to obtain information about a workpiece’s 3-D geometry and material properties. XCT systems work by generating a beam of x-rays that propagate through the workpiece and are then measured by a detector to generate a radiograph. As the workpiece rotates, many radiographs are generated. Through a computationally intense reconstruction process, the radiographs are used to generate a 3-D voxel model of the workpiece. Demand for XCT for dimensional metrology has increased along with the advent of processes such as additive manufacturing which yield parts with more complex internal geometries. Using the free, open-source ASTRA toolbox for MATLAB, we are developing simulations to help quantify the effects of uncorrected instrument geometry errors found in CT systems by looking at the influence the errors have on sphere form and sphere center-to-center measurements. We hope to use this tool to further validate the single-point ray tracing method developed at NIST. ASTRA’s modular design allows any step and variable in the simulation to be changed. Using this feature, we plan to implement error in the forward projection, such as a detector shift, and generate a reconstruction. The reconstructed model will then show the error as a sphere form or location error. The results of our work thus far have yielded a code capable of generating sphere artifacts and reconstructions based on a specified set of input variables that represent XCT parameters. This code will not only serve as a validation tool for the ray-tracing method, but also as a framework and tool for the validity of future simulations. This work will help support the ongoing standards development efforts of ISO 10360-11 and future revisions of the ASME B89-4-23, which are both standards for the performance evaluation of XCT systems.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Alessandro Rizzoni

Academic Institution: Western Michigan University

Major: Electrical Engineering

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): I plan to attend graduate school to study electronics, control systems, and electromagnetic design.

NIST Laboratory, Division, and Group: PML, MND, Photonics and Optomechanics Group

NIST Research Advisor: Vladimir Aksyuk, Alexander Yulaev, Chad Ropp

Title of Talk: Optimal Design of Fiber to Waveguide Facet Coupler Geometries Using the Finite Element Method

Abstract:

Photonic Integrated Circuits (PIC's) are currently under development for applications in atomic physics where optical interrogation is required. In such experiments, matter may be subjected to optical frequency electromagnetic radiation in order to perform various measurements. Lasers can be used to generate radiation of sufficient intensity and concentration, but to precisely direct and manipulate the light optical fiber and a PIC are used. The light is guided by optical fiber to the PIC as a fiber mode, and requires mode conversion to efficiently excite the desired waveguide mode. To improve coupling of the fiber mode to a waveguide mode, a facet coupler is required. Such a device consists of a tapered waveguide connecting two ports, and bidirectionally converts from one mode to another. In order to investigate more efficient methods of optical coupling, a working model of a rectangular waveguide was developed to compare against experimental results, then a series of simulations and analyses in COMSOL Multiphysics and MATLAB were performed to investigate the effect of various geometric deformations. It was found that the laboratory measurements of 3 dB for the transmission losses of the 150 x 100 nm rectangular waveguide were reasonable as the simulation yielded a value of 1.25 dB for the same size waveguide, showing room for improvement in the laboratory. To improve transmission, a model of a tapered facet coupler is under development. Assuming that a long enough taper can operate adiabatically, several geometries are being considered to determine the optimal shape to maximize transmission. The tapered waveguide geometry shows promising efficiency, and further developments are expected to be realized through the implementation of deformation-based optimization algorithms as well as continued iterative design. Studies investigating the impact of mesh element size, cladding thickness, system size, and boundary conditions were also performed, and a procedure for the modeling of waveguide structures was developed. This work serves as a starting point for further development of optimal facet coupler geometries, and could be readily adapted for the development of other waveguide geometries.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Jared Schwartz			
Academic Institution:	University of Maryland	**Major:**	Physics
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Graduate School for Physics		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Atomic Spectroscopy Group		
NIST Research Advisor:	Gillian Nave		
Title of Talk:	Branching Fractions and Oscillator Strengths in Singly Ionized Chromium		

Abstract:

Spectral lines of singly ionized Chromium (Cr II) are present in the spectra of many astrophysical objects, including stars, the interstellar medium, and nebulae. However, interpretation of these spectra is hampered by a lack of atomic data for these lines, including atomic transition probabilities. Such transition probabilities can be measured by combining a measurement of the relative intensities of all spectral lines from a particular upper level with the lifetime of that level. While the NIST Atomic Spectra Database contains over 4000 spectral lines for Cr II below 350 nm, fewer than 300 transition probabilities for these lines have been measured. In order to catalog the transition probabilities of Cr II, archived spectrographic data recorded by a NIST FT700 vacuum ultraviolet Fourier transform spectrometer from chromium and argon hollow cathode lamps were analyzed. Using a specialized program to plot and analyze atomic spectrographic data, gaussian profiles were fit to spectral lines at known transition frequencies. An intensity correction of the sampled lines was then applied by dividing the fitted lines by the response curve yielded from a deuterium hollow cathode lamp. The intensity-corrected lines were then sorted by their upper levels and their intensities were normalized into branching fractions using another specialized python program. By combining these branching fractions with known lifetimes for the upper levels of Cr II, a table of the transition probabilities was constructed for 15 upper levels of Cr II.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Christopher Sherald		
Academic Institution:	University of Kansas	**Major:**	Physics
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Get a PhD in Applied or Condensed Matter Physics and pursue a career in industry		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Atom Scale Device Group		
NIST Research Advisor:	Richard Silver		
Title of Talk:	Modeling Devices for Atom-based Silicon Quantum Electronics		

Abstract:

This research project is focused on the design and fabrication of atom-based silicon transistors. Key to the design of this electronic structure is the utilization of advanced hydrogen-lithography to place individual dopant atoms in a silicon matrix. The purpose of the devices is to shuttle single electrons across an array of silicon quantum dots. Due to the scale of the devices, tuning the capacitance, and thus potentials, of the quantum dots to facilitate electron transport, affects the potentials of nearby dots and thus, is not a simple process. By creating sample models using the FreeCAD software, and by utilizing a capacitive modeling program, we can tune the gate and capacitive control of the device as desired and better guide the design process.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Myles Sherman

Academic Institution: California Institute of Technology **Major:** Physics

Academic Standing (Sept. 2021): First Year PhD Student

Future Plans (School/Career): Pursuing PhD in Physics, conduct research in experimental astrophysics and instrumentation

NIST Laboratory, Division, and Group: Physical Measurements Lab, Quantum Measurement Division, Applied Electrical Metrology Group

NIST Research Advisor: Dr. Richard Steiner

Title of Talk: Characterization of Fluke 8588 for Digital Power Measurement

Abstract:

The immediate purpose of this project is to characterize the Fluke 8588 Digital Multimeter's (DMM) behavior when measuring low frequency (10 Hz – 1 MHz) AC voltage and current from digitized data. The process of calculating the root mean squared (RMS) voltage of AC signals using optimized discrete samples is known as Swerlein's algorithm. The goal is to evaluate the error in measurements produced using this technique, determine possible sources of this error in the electronics or implementation, and create applicable correction factors to extend the DMM's range of accuracy (within 0.01%). The reconstruction step can be done either by fitting a sum of harmonic sine waves to the samples (4-parameter sine fit) or by evaluating the Fast Fourier Transform (FFT), and an additional goal is to compare the effectiveness of each method. Errors in the data can be dependent on a number of parameters including input frequency, sample rate, and aperture time. Errors that already have well-defined correction factors, such as for aperture time and lowpass filter bandwidth, are applied to the data and evaluated for their ability to correct the signal relative to the calibrator output. The remaining error is then fit to possible characteristic equations, and attributed to properties of the F8588 or calibrator. Initial data was taken with respect to sample rate and frequency to determine a valid test parameter space. Then, RMS voltage data taken in each DMM range over the relevant frequencies was processed with known corrections, and the remaining error was shown to have higher order behavior at high frequencies, with a 'resonance' near 5 kHz in some cases. Further knowledge of the calibrator and DMM electronics is needed to fit a characteristic equation to this error. In conclusion, while a method for determining the error was implemented, more information about the source of the error is needed to develop a correction factor. The sine fit and FFT methods must be investigated further as well to account for errors they introduce. Once the DMM is characterized, the overall goal is to utilize it to calibrate AC outputs from calibrators and more accurately measure the harmonic content of AC power distorted by non-linear loads like LED's.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Catherine Silver

Academic Institution: Cornell University

Major: Chemistry

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Pursue a graduate degree in Chemistry

NIST Laboratory, Division, and Group: PML, Sensor Science Division, Surface and Interface Metrology Group

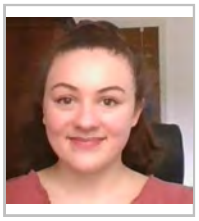
NIST Research Advisor: Alan Zheng

Title of Talk: Optimization of Low and High pass Cutoff Parameters for Firearm Population Statistics

Abstract:

Within the criminal justice system, there are several automated algorithms being utilized to compare forensic evidence (e.g. DNA and fingerprints). NIST have been developing objective algorithms for firearm and toolmark comparisons for the past decade. The primary goal of this research is to provide forensic examiners with an objective similarity metric and associated weight of evidence estimations that can be used in court testimonies. When a semi-automatic firearm is fired, the cartridge case is ejected, and is left with an impression of the firing pin and breech face. These are some of the unique toolmarks that examiners use to identify the source firearm. The NIST algorithms developed to quantify the similarity of these toolmarks are Congruent Matching Cells method (CMC) and the Areal Cross Correlation Function (ACCF). The CMC method breaks up the topography image into an array of square cells. Then, with specified thresholds and parameters, these cells are matched to corresponding areas on the questioned cartridge case. Similarly, the ACCF method compares the entire measured topography area.

My project consisted of optimizing correlation parameters to maximize the separation between known matching and known non-matching populations of scores. Additionally, the Kruskal Wallis test was used to test if there were any significant differences between populations due to modifying a parameter. The primary parameters of interest in my research are the Gaussian Regression low and high pass filter cutoffs. The Gaussian Regression filter is used to extract the toolmarks of interest by removing long wavelength waviness and short wavelength noise from the data. To optimize these two filters, correlations were conducted with a combination of Gaussian Regression high and low pass cut offs using a full factorial design. To analyze the data outputted from the surface correlator software, an R script was written to display basic statistics, along with graphs to help determine the degree of separation between the known match and known non-match populations. The presentation will display the optimal parameters that provide the greatest separation in CMC and ACCF scores for known matching and known non-matching populations.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name:	Katherine Slattery		
Academic Institution:	University of Cincinnati	**Major:**	Physics, Mathematics
Academic Standing (Sept. 2021):	Graduated Spring 2021		
Future Plans (School/Career):	Graduate school in Physics, pursue a research career in government or industy		
NIST Laboratory, Division, and Group:	Physical Measurement Laboratory, Quantum Measurement Division, Quantum Optics		
NIST Research Advisor:	Zachary Levine		
Title of Talk:	Conditions for a Single Photon Echo		

Abstract:

The development of photonic quantum memory in rare earth ion crystals using the atomic frequency comb protocol relies on photon echoes. Modelling these photon echoes provides insights which may enhance future experimental efforts. In this work, we model the dielectric function of the crystal to determine how this affects photon echoes. We illustrate the effect that altering the ratio of free spectral range to full width at half maximum (finesse) of dielectric function has on the photon echo. When the finesse is much greater than one, photon echoes go on for a long time. When finesse is approximately equal to one, there are a small number of photon echoes, and perhaps only one photon echo, a necessary feature for high efficiency quantum memory. As an aside, we also present a few notes on the Hamiltonian for Pr:YSO which may be used as a quantum memory system.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name:	Ross Snyder		
Academic Institution:	University of Colorado Boulder	**Major:**	Physics
Academic Standing (Sept. 2021):	Graduated		
Future Plans (School/Career):	Graduate School/Research		
NIST Laboratory, Division, and Group:	PML, Boulder, Quantum Nanophotonics		
NIST Research Advisor:	Krister Shalm		
Title of Talk:	Creating a quantum toolbox for the web		

Abstract:

Some of our NIST web-based tools need functions that can characterize and calculate common measures of entanglement between quantum states of light called photons. Quantum entanglement is a phenomenon that occurs between two or more quantum states, and it refers to the fact that these states are connected, even if they are spatially separated. At NIST, we generate entangled photons and use them for several metrology applications.

To characterize quantum states and provide measures of entanglement, we chose a programming language called Rust because it works well with web-based user interfaces. However, there is no library of convenient quantum functions in Rust that exists yet.

In my talk, I will discuss my creation of a quantum library in Rust, and illustrate how some of these functions can be used to calculate the properties of quantum states that are represented as a density matrix. A density matrix can characterize how mixed or pure quantum states are, and it is useful in experiments because it quantifies the purity of polarization encoded photonic qubits. This library will be a convenient tool for calculating needed properties of quantum states. We plan to publish this library as an open-source package that anyone can use. This package will be continuously updated to provide even more convenience for the community.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name:	Cassie Stoffer		
Academic Institution:	Willamette University	**Major:**	Physics
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Attend graduate school		
NIST Laboratory, Division, and Group:	Physical Measurement Lab, Applied Physics Division, Magnetic Imaging Group		
NIST Research Advisor:	Karl Stupic, Michele Martin		
Title of Talk:	Investigating Temperature Changes in Low Field DNP		

Abstract:

Nuclear magnetic resonance (NMR) is a process that uses magnetic fields to excite the spins of atomic nuclei in a sample, resulting in an electromagnetic signal. At low fields (< 1 T), NMR becomes more cost efficient and portable but can suffer from low signal to noise ratios (SNR). Dynamic nuclear polarization (DNP) is a technique that offers a desired increase in SNR by exciting electron transitions in samples containing free radicals. The resulting low field NMR spectrum is enhanced due to a transfer of polarization from excited electrons to the nuclei being studied. A digital electron paramagnetic resonance (EPR) system was developed that has the potential to determine the necessary frequency for electron excitation in DNP experiments. This system will allow radicals beyond those explored in this project to be studied via DNP.

The high power radiofrequency applied throughout a DNP experiment produces heat that can change the temperature of a sample. Because magnetic resonance is a non-destructive technique, it is used in a number of applications with highly sensitive or valuable samples. Thus, it is of great value to study temperature changes that occur throughout an experiment. This project investigated the impact such temperature changes have on the enhancement of DNP spectra. Using different concentrations of the free radical CTPO, DNP experiments were conducted at different excitation powers. For a specified sample concentration and power, the amplitude of the DNP spectrum was recorded at varying electron excitation times. The data was processed by converting the recorded amplitudes into enhancements and observing the impact temperature had on these enhancements.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Ethan Swagel

Academic Institution: Brown University

Major: Mathematical Physics

Academic Standing (Sept. 2021): Junior

Future Plans (School/Career): Graduate school

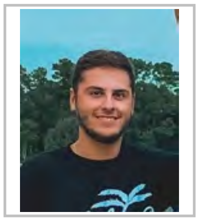
NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Nanoscale Device Characterization Division, Nanoscale Spectroscopy Group

NIST Research Advisor: Jared Wahlstrand

Title of Talk: Analysis of Complex Multidimensional Optical Spectra by Linear Prediction

Abstract:

Multidimensional coherent spectroscopy (MDCS) is a versatile technique for exploring light-matter interactions in semiconductor nanostructures and can provide a more complete understanding of photonic and electronic phenomena to be exploited in optoelectronic applications. MDCS is based on multi-pulse time-domain third-order nonlinear optical spectroscopy, known as four-wave mixing, from which the signal is converted into multiple frequency dimensions to separate complex and overlapping spectral contributions. The optical signal is typically analyzed in the frequency domain through a discrete Fourier transformation (DFT), which computationally deconstructs the temporal oscillations into multidimensional peaks representing the constituent contributions of sinusoids at each frequency. When peaks are located at nearby frequencies, weaker features of interest can be obscured by the tails of stronger peaks. Here, linear prediction from singular value decomposition (LPSVD) is implemented, which uses a non-iterative linear fitting procedure to fit the time-domain signal to a model of the sum of damped sinusoids. Because the fitting is linear, it is not necessary to guess initial fitting parameters, as in the more common method of nonlinear fits. We apply LPSVD to the analysis of zero-, one-, and two-quantum two-dimensional spectra from a III-V semiconductor microcavity in order to separate the strong exciton-polariton response from weaker biexciton features. It is shown that LPSVD reduces noise, eliminates distortions inherent in DFT algorithms, and isolates and allows for the analysis of weak features of interest. Additionally, we show that LPSVD handles highly non-ideal peaks without requiring a predetermined analytical model, as in nonlinear fitting, by fitting non-Lorentzian peaks with multiple Lorentzians. Applying this method to the semiconductor microcavity will allow for precise determination of nonlinear optical interactions in these complex devices.



SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: James Vouzikas, Jr.

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

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Graduate School/Professional Engineer

NIST Laboratory, Division, and Group: Physical Measurement Laboratory, Quantum Measurements, Mass and Force Group

NIST Research Advisor: Dr. Michael Gaitan

Title of Talk: Pendulum and Rotational Calibration Comparison of Three-Axis Gyroscopes

Abstract:

A three-axis accelerometer and gyroscope has the ability to measure acceleration and rotation changes occuring about each axis in a cartesian system. Over the past 11 weeks, we have developed a unique approach to calibrate the accelerometer and gyroscope integrated on an Adafruit Feather nRF52840 Sense. This device, capable of of sending accleromoter and gyroscope data via bluetooth, was studied and analyzed using software packages including the Arduino IDE, Python 3, and Excel. A new calibration approach for calibrating gyroscopes was developed using a pendulum as the exitation source. The device was calibrated and compared to a claibration using a 2-axis angular position and rate table with constant rotation exitation. Static conditions were also considered in order to determine the offset of the device and ultimately to quantify its sensitivity. This report will focus on the comparison of the calibration using the pendulum and the rate table. As each device can not be manufactured exactly the same, the team aimed to compare readings of offset and sensitivity against each other and against the manufactures data as well.

SURF Student Colloquium

NIST – Gaithersburg, MD
August 2-6, 2021

Name: Kendall Zammit

Academic Institution: Appalachian State University

Major: Chemistry

Academic Standing (Sept. 2021): Senior

Future Plans (School/Career): Chemistry Professor

NIST Laboratory, Division, and Group: Gaithersburg, Physical Measurement Lab, Nanoscale Imaging Group

NIST Research Advisor: Yaw Obeng

Title of Talk: Mining of Solder Joint Reliability Data to Identify Possible Precursors to Catastrophic Failure

Abstract:

Solder joint failures found in electronic systems fall into 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 /hard 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 an thermally controlled chamber cycling between 0 ℃ and 100 ℃, while monitoring the electrical properties of the joints. Comparing the cycle number, corresponding temperature, and microwave signal return loss (S11) output, distinct breaks were observed in the S11 vs time plots. These break points appear to relate to different events occurring in the solder joints prior to complete failure. While we do not fully understand the physico-chemical nature of these events, they possibly include the recrystallization of the solder joint alloy. Further research is ongoing into further understand the events seen during the overall failure picture.

SURF Student Colloquium

NIST – Boulder, CO
August 2-6, 2021

Name: Laura Zhou			
Academic Institution:	Yale University	**Major:**	Physics
Academic Standing (Sept. 2021):	Senior		
Future Plans (School/Career):	Graduate school in physics		
NIST Laboratory, Division, and Group:	Physical Measurements Laboratory, Time and Frequency Division, Optical Frequency Measurements Group		
NIST Research Advisor:	Tara Fortier		
Title of Talk:	Developing a unified statistical framework for the analysis of atomic clock data		

Abstract:

Optical atomic clocks are ultraprecise systems that define time from the oscillations of electronic quantum transitions. Currently, frequency comparisons between optical clocks at different National Metrology Institutes, used to characterize clock accuracy, stability and reproducibility, can only be compared "on paper" as published values. The comparisons are reported as unitless frequency ratios, permitting precisions beyond the limits of the current SI standard. The ratio of different atomic clock transition frequencies help to support a wide variety of applications. For instance, international comparisons support realization of the international time standard. Additionally, comparisons of different atomic clock species can be used to test fundamental physics, such as models of dark matter.

As the precision of frequency ratio measurements continues to improve, it will be important to evaluate the performance of traditional methods of ratio data analysis. Formally accepted values of frequency ratios are calculated based on periodic studies performed at many different laboratories. It has been documented that in these scenarios that when the individual studies of frequency ratios are compiled, the reported values exhibit scatter beyond what is expected based on their accuracies and stabilities. While there exist several statistical methods for resolving the measurement uncertainty within over scattered data, we lack a standard framework for determining which methods are preferable for a given instance of observed ratio data. Within this project, we identify popular statistical models of inconsistent frequency ratio data. In particular, we compare traditional methods of analysis to a more comprehensive statistical model which incorporates our prior beliefs about the ratio variability. We evaluate the performance of the methods by applying them to simulated clock frequency ratio data and compare the accuracy of the summarizing statistics. The ratio data simulations vary in noise characteristics, degree of scatter, and number of measurements, reflecting features of frequency ratio datasets reported in the literature. Our results are a step toward establishing a standard procedure for analyzing clock frequency ratio data.