2022 Student Symposium
Project Descriptions

Los Alamos
NATIONAL LABORATORY

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OLIVIA ASHER

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF GEORGIA
GROUP: B-11
MENTOR: HAU THI BICH NGUYEN
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: ENZYME ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26482

OPTIMIZING ENZYMES FOR DIGESTING PLASTICS

Plastic waste proliferates for thousands of years, negatively impacting environmental and human health. Ideally, we could utilize the benefits of plastic without producing harmful waste. To do this, we must find new methods of breaking down plastics. Several plastic-digesting enzymes found in bacteria have been identified and characterized. The most well-known of these enzymes are IsPETase, LCC, and PHL7, which break down polyethylene terephthalate (PET), the type of plastic used in most food packaging. In this project, we use directed evolution to improve enzyme activity, expression and thermostability of LCC enzyme. The enzymes we create have potential to be used to digest post-consumer plastic waste in the future.

ABDUL-RAHMAN AZIZOGLI

PROGRAM: UNDERGRADUATE
SCHOOL: NEW JERSEY INSTITUTE OF TECHNOLOGY
GROUP: B-11
MENTOR: RAMESH JHA
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: PROTEIN ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26780

PERTURBING GLOBAL REGULATION IN P. PUTIDA FOR INCREASED MUCONATE PRODUCTIVITY

The bacterial Pseudomonas putida strain KT2440 has been genetically engineered to utilize carbon sources to produce high value commodity chemical cis,cis-muconate. Muconate production from renewable sugars is of interest to replace the current production from petrochemical feedstocks. To achieve high titer, rate and yield, we targeted a global regulator called Catabolite Repression Control (crc) protein, which regulates many of the genes involved in carbon substrate metabolism. The complex structure of crc has been elucidated in a closely related organism, P. aeruginosa. In this project, the Rosetta modeling suite is used to predict mutations in crc, construct a crc library and select for high muconate producers using LANL invented biosensor technology.

DANIELA FLOREZ PINEDA

PROGRAM: GRADUATE
SCHOOL: TULANE UNIVERSITY
GROUP: T-6
MENTOR: CARRIE MANORE

DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: EPIDEMIOLOGY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27241

ASSESSING THE RISK OF DENGUE OUTBREAKS ACROSS CONTINENTAL BIOMES IN BRAZIL

Dengue is a mosquito vector-borne disease that causes an estimated of 390 million new infections every year. The environmental temperature has been identified as a key driver of these annual dengue case counts. However, the interaction between dengue transmission and temperature exhibits a complex non-linear relationship that has not been well outlined in existing theoretical frameworks. We focus our study on characterizing temperature-dependent dengue risk using a SEIR-type model and analyze its behavior across tropical eco-zones. Because of their well-differentiated ecological diversity, we have selected Brazil continental biomes to better illustrate the effects of spatial and temporal temperature heterogeneity on dengue dynamics.

CINLONG HUANG

PROGRAM: UNDERGRADUATE
SCHOOL: UC BERKELEY
GROUP: B-10
MENTOR: SOFIYA MICHEVA-VITEVA
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: PATHOGEN BIOLOGY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27185

DEVELOPING MEDICAL COUNTERMEASURES TO CHOLINERGIC CRISIS IN HUMAN MOTOR NEURONS

While there are no universally effective medical countermeasures against the diverse set of nerve toxins, chemical warfare agents (CWA) continue to pose a great threat to the Armed Forces and civilians. Our primary scientific objective is to identify novel molecular targets for development of broad-spectrum prophylactics or tissue regenerative antidotes to CWA-induced injuries. We have developed human motor neurons (MNs) from adult induced pluripotent cells and have subjected them to various concentrations of ACh and POXE to induce cholinergic crisis. Based on our findings, inhibitors to VDAC, AChR, and Ca-voltage channels can serve as medical countermeasures (MCM) to cholinergic crisis. To test the effect of potential MCM, we have established a fluorescent-based Ca2+-flux assay.

MAKAELA JONES

PROGRAM: POST BACHELORS
SCHOOL: NEW MEXICO STATE UNIVERSITY
GROUP: C-PCS
MENTOR: JESSICA KUBICEK-SUTHERLAND
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: BIOLOGICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26594

USING BIOPHYSICAL TOOLS TO EXPLORE NUCLEIC ACID HYBRIDIZATION FOR DIAGNOSTICS

Nucleic acids contain genetic information that encompasses the biological instructions for living organisms and can be detected to identify pathogens. The detection of nucleic acids depends on hybridization of complementary strands, which often requires highly purified samples and is not suitable for fieldable diagnostics. We are using Raman spectroscopy and isothermal titration calorimetry (ITC) to study nucleic acid vibrations and the thermodynamics of hybridization. We constructed a simple Raman spectrometer to directly detect nucleic acids. Because viruses mutate rapidly, we used ITC to assess the effects of nucleic acid mismatches on hybridization efficiency. Our Raman sensor has the potential to support a robust and rapid diagnostic tool sensitive enough to detect viral mutations.

TRENT LLEWELLYN

PROGRAM: POST BACHELORS
GROUP: C-PCS
MENTOR: JESSICA KUBICEK-SUTHERLAND
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: IMMUNOLOGY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26694

A COMPARATIVE META-ANALYSIS OF CYTOKINE PROFILES BETWEEN RESPIRATORY DISEASES

Cytokines are useful biomarkers for detecting the progress and severity of a disease. We wanted to investigate cytokines as a diagnostic tool to distinguish diseases with similar sites of infection and symptoms. We conducted a meta-analysis of cytokine expression levels between infected and healthy individuals of three different upper respiratory diseases: COVID-19, influenza A, and RSV. We found six elevated cytokines, IL6, TNF-α, IFN-γ, IL18, CXCL10 and IL10, shared between disease groups. CXCL10 was significantly elevated in COVID-19 infections compared to influenza A infections. Our study shows most elevated cytokines are shared across disease groups but the difference in CXCL10 could indicate COVID-19 recruits more macrophages and delays adaptive immune response.

LEXY LUJAN

PROGRAM: UNDERGRADUATE
SCHOOL: ARIZONA STATE UNIVERSITY
GROUP: B-11
MENTOR: HAU THI BICH NGUYEN

DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: PROTEIN ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26747

ENGINEERING NEW SPLIT FLUORESCENT PROTEIN SYSTEMS FOR MULTIPLEXED LABELING

Split green fluorescent protein has been used widely in modern cell biology to track protein translocation, monitor protein solubility and aggregation, detect protein-protein interactions. Our team is particularly interested in using split fluorescent proteins for large scale labeling of proteins in living cells and as detection reagents for diagnosis test kit. In order to improve the labeling process, several sets of efficient split fluorescent proteins that do not cross-react are needed. We are developing a new 3-body split green fluorescent protein (from strawberry anemones) and 3-body split cherry fluorescent protein (from sea anemones) by directed evolution to enable multiplexed labeling with our existing split green fluorescent protein from jelly fish.

AENGUS MCGUINNESS

PROGRAM: HIGH SCHOOL
SCHOOL: SANTA FE HIGH SCHOOL
GROUP: B-10
MENTOR: BLAKE HOVDE
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: BIOINFORMATICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26719

CRISPR OFF-TARGET DAMAGE ANALYSIS

CRISPR Cas-9 has revolutionized the field of genomics by providing a powerful tool for genome editing that has ramifications for fields ranging from Microbiology to Oncology. However, CRISPR Cas-9's off-target mutation rate is largely unknown which limits its applications. The CODA (CRISPR Cas-9 Off Target Damage Analysis) pipeline aims to use k-mer counts for an unbiased search of the entire genome for off-target edits. Through comparing k-mer counts before and after the CRISPR Cas-9 editing occurred, CODA is able to isolate k-mers of interest that could be indicative of an edit. The reads from these k-mers are then aligned to a reference genome and filtered to reduce the false positive rate. Preliminary results have shown that somatic mutations may mask the presence of off-target events.

GILLIAN MCMAHON

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF CALIFORNIA, SAN DIEGO
GROUP: B-11
MENTOR: JENNIFER FOSTER HARRIS
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: SPECTROSCOPY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-19-29407

FULL SPECTRUM MICROFLUIDIC FLOW CYTOMETRY

We are creating a low-cost, microfluidic flow cytometry system that will measure up to 21 different parameters of individual cells from samples as small as a few hundred microliters. Unlike conventional flow cytometers that measure 10's of parameters and use up to six lasers, this system will use only two lasers and any dye that is excited by a 408 or 532 nm laser. In contrast to current flow cytometers, the system measures the full wavelength range of the emission spectra at a resolution of 1-2 nm. The increased capability of this system is especially applicable to studying malaria because it will measure multiple cell markers from a single sample, it will be able to test on a small sample, such as those obtained from the anemic children, and it has the potential to be field-deployable.

ABIELA MEEK

PROGRAM: UNDERGRADUATE
SCHOOL: UTAH STATE UNIVERSITY
GROUP: B-11
MENTOR: NILUSHA APPUHAMILAGE
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: BIOFUELS AND BIOPRODUCTS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26593

EVALUATING CYANOPHYCIN PRODUCTION IN CYANOBACTERIA

With the current volatility of the oil market and environmental implications of oil production, crude oil replacements are more necessary than ever. Cyanophycin (CP), an amino acid based polymer naturally produced in cyanobacteria under nutrient limited conditions, presents a promising solution, as it can be transformed into polyaspartate, a green, biodegradable polyacrylate replacement. In this project, we will evaluate CP accumulation in the cyanobacterial strain, Synechosystis sp. 6803, at different stages of the growth cycle and report on CP levels. To evaluate CP production, we will develop methods for CP extraction from Synechosystis sp. 6803 and CP quantification by NMR. If successful, this research will detail how CP productivity can be optimized in cyanobacteria.

SHEPARD MOORE

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF NEW MEXICO
GROUP: C-PCS
MENTOR: HARSHINI MUKUNDAN
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: BIOMEDICAL SCIENCE/ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26550

EFFECTS OF URANIUM OXIDES ON HUMAN LUNG CELLS

There are few studies on the specific, long-term health consequences of aerosolized radioactive particulate exposure to the human respiratory system. Given the threat of radioactive events and other environmental/occupational exposures, there needs to be a systematic study on how internal human tissues respond to inhaled radionuclide particulates. This work is currently investigating the in vitro effects of well characterized (<10 μm) depleted uranium (DU), natural uranium (NatU) oxide particles in human lung cells, with future directions to use highly enriched uranium (HEU). Evaluating cytotoxic effects and biomarker changes at various levels of enrichment provides an integrated approach to distinguish the radiological from the chemical toxicity of uranium exposure.

KANE MOSER

PROGRAM: POST BACHELORS
SCHOOL: BARD COLLEGE
GROUP: B-10
MENTOR: ANDREW BARTLOW

DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: ECOLOGICAL HEALTH SECURITY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-25785

CULEX SPP. MOSQUITO LIFE HISTORY TRAITS AND APPLICATIONS IN DISEASE MODELING

Culex mosquitoes, the primary vectors for West Nile virus (WNV) in the U.S., are undergoing rapid range expansions due to climate change, but there is high heterogeneity in how each species is responding. This is due to variation in life history traits, which need to be included in disease forecasting models. We reviewed the effects of temperature on immature development rate, egg viability, survival to adulthood, oviposition, and adult lifespan for four Culex species. We found that different traits and species responded differently to temperature. We created temperature-based WNV R0 maps for each Culex species and identified data gaps. Understanding species and trait relationships with the environment is critical for accurate predictions of mosquito population dynamics and disease risk.

BAILEE NASISE

PROGRAM: UNDERGRADUATE
SCHOOL: UC BERKELEY
GROUP: B-11
MENTOR: THOMAS GROSECLOSE

DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: ENZYME ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26872

HIGH-THROUGHPUT ENZYME ENGINEERING FOR DEGRADATION OF PLASTIC WASTE

Recently, researchers have discovered new ways to degrade the artificial plastic polluting the earth and devastating its ecosystems. Enzymes from bacteria and fungi have been found to digest these harmful plastics. However, these enzymes are not optimized for large-scale industrial recycling, and therefore they must be engineered further. For my project, I have chosen to study a novel enzyme that was recently reported to digest polyethylene terephthalate (PET) at high crystallinities. To make this enzyme more thermostable and possess stronger plastic degrading properties, necessary for its industrial use, I will use directed evolution, followed by screening, to demonstrate how this enzyme's function can be improved and ultimately restore the planet.

ANJALI PARANDE

PROGRAM: UNDERGRADUATE
SCHOOL: COLUMBIA UNIVERSITY
GROUP: B-10
MENTOR: KUMKUM GANGULY
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: BIOSCIENCES
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26998

A NOVEL APPROACH TO UNDERSTAND THE EVOLUTION OF DRUG-RESISTANCE IN LUNG CANCER

Lung cancer is the leading cause of cancer mortality in the US with >130,000 deaths per year. The development of resistance to chemotherapeutics is a main reason for treatment failure. Using a genome wide CRISPR/Cas9 activation screen, we identified genes conferring resistance to chemotherapeutic Erlotinib. In KGI, we transduced a non-small cell lung cancer cell-line with a library of 74,000 guide RNAs against promoters of all human genes. At LANL, analysis of a genome-wide deep sequencing of Erlotinib resistant cells yielded 45 drug resistant genes—8 of which were highly expressed. We transfected HCC827 cells with 3 plasmids containing genes SPATA3145, MAPKAP1 and SH3D19 to confirm resistance to Erlotinib. These results will help us to design future assays for drug screening.

DANIELA RODRIGUEZ-CHAVEZ

PROGRAM: UNDERGRADUATE
SCHOOL: CORNELL UNIVERSITY
GROUP: A-1
MENTOR: MORGAN GORRIS
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: ECOLOGICAL MODELING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26014

ASSESSING THE CORRELATION BETWEEN BIRD MIGRATIONS, CLIMATE, AND WEST NILE VIRUS

West Nile virus (WNV) is the largest cause of mosquito-borne illness in the US and primarily circulates between birds and mosquitoes. Passerine birds, such as American Robins and Blue Jays, are amplifying hosts and can act as super-spreaders of the disease, especially along migration routes. With climate change causing earlier, warmer springs that are changing the timing of bird migration, understanding how changes in seasonal patterns of bird migration affect outbreaks of WNV will be crucial for public health. Focusing on the U.S., I curated a list of bird species that are especially competent at transmitting West Nile virus. I mapped bird migration patterns with corresponding weather data and tested for correlations between spring bird migrations, weather data, and WNV case outbreaks.

NELSON RUTH

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF OREGON
GROUP: B-10
MENTOR: MIGUN SHAKYA
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: BIOSURVEILLANCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27124

WHAT'S LURKING IN YOUR SEWER? ASSESSING MICROBIAL DIVERSITY USING PUBLIC DATA

Monitoring wastewater can be an effective method to track and detect disease outbreaks. Biosurveillance has been used for decades, but its importance has resurged due to its utility for predicting COVID-19 spikes in a community. For this low-cost and non-invasive method to become routine, the poor characterization of wastewater's microbial diversity must be addressed. Here, we remedy this bottleneck by aggregating and analyzing publicly available data from across the world. We used the raw reads to assemble contigs, which were further processed for characterization of taxonomic and functional content of wastewaters. Our results provide a detailed comprehensive description of global wastewater dynamics and created a specific reference database for future routine wastewater monitoring.

DANA URBATSCH

PROGRAM: UNDERGRADUATE
SCHOOL: ARIZONA STATE UNIVERSITY
GROUP: B-10
MENTOR: SHAWN STARKENBURG
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: MOLECULAR BIOLOGY
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27063

Normalizing SARS-CoV-2 detected in wastewater

The monitoring of SARS-CoV-2 through individual testing is subject to inaccuracies. Due to fecal shedding of SARS-CoV-2, wastewater can be analyzed in order to detect varying levels of the virus within a community. Pepper Mild Mottle Virus is present consistently in human fecal matter, and can be used to normalize the amount of SARS-CoV-2 detected. In this experiment, the amount of SARS-CoV-2 in the wastewater sample was compared to the amount of PMMoV present. Wastewater samples were separated into three fractions: direct wastewater, a solid pellet, and filter paper extract. A qPCR test was used on the extracted RNA from each fraction to detect the relative amount of SARS-CoV-2 and PMMoV copies in each sample. The amount of SARS-CoV-2 was successfully normalized to the amount of PMMoV.

SEYCHELLES VOIT

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF FLORIDA
GROUP: B-10
MENTOR: SHAWN STARKENBURG
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: BIOLOGICAL SCIENCE
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27247

DISCOVERING ORGANIC FLUORESCENCE SIGNATURES IN A PLANETARY-EXPLORATION CONTEXT

Radiation laden Mar’s sub-surfaces are extremely interesting from an astrobiology perspective. Mar's subsurface may harbor life and biosignatures from this life might be brought up to the surface. To detect camouflaged signatures of life, one can study earth’s ‘extremophiles’3—organisms growing in extreme cold, dehydration, vacuum, acidity, mineral-rich conditions or radiation. We irradiated biomaterials in the well-characterized proton, Gamma and neutron beams at the pRad facility, RP and ICE House respectively to analyze.

ADALEE WITT

PROGRAM: UNDERGRADUATE
SCHOOL: OREGON STATE UNIVERSITY
GROUP: B-11
MENTOR: CESAR ESQUER
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: BIOMANUFACTURING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27238

ALGINATE HYDROGELS AND CYANOBACTERIAL COMPOSITES AS RENEWABLE BIOMATERIALS

The LDRD-DI project “Biotechnology for Regional Climate Resilience” seeks to develop technologies that address the causes and effects of climate change. As part of this project, I will experiment with hydrogel matrices mixed with cyanobacterial biomass as an innovative material precursor for biomanufacturing applications that can replace current, polluting cements. Specifically, I will evaluate mixing proportions of calcium alginate hydrogels, including a cyanobacterial and nutrient component, to optimize bacterial activity and calcium deposition. Ultimately, this type of material has the potential for real-world applications, such as for environmentally friendly housing, bioinks for 3-D printing, or cement-repair paste, in order to reduce climate change-causing CO2 emissions from cement.

KAYLEY YOU MAK

PROGRAM: POST BACHELORS
GROUP: B-10
MENTOR: BLAKE HOVDE
DISCIPLINE: BIOLOGICAL SCIENCE
SUBJECT AREA: BIOLOGY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26461

CHARACTERIZING MICROBIAL COMMUNITIES IN LONG-TERM ALGAL PONDS ACROSS SITES

The growing importance of biofuels has led to research focusing on the effects of the microbial community. Algal-bacterial consortia have demonstrated synergistic mutualisms, as well as pestilent and predatory interactions. To optimize industrial-scale algal growth, we are characterizing the long-term stability and the effect of location on the microbial community in outdoor algal ponds. Since the Fall of 2020, weekly samples were collected from 3-4 continuously cultured algal ponds at three sites: San Diego, CA; Las Cruces, NM; and Kailua-Kona, HI. The pond-level community was 16S/18S amplicon sequenced. The replicate pond communities differed only slightly, but varied by location, indicating that the local fauna will influence algal growth and therefore biofuel yields.

CHEMISTRY

LOGAN AUGUSTINE

PROGRAM: DOE SCGR FELLOW
SCHOOL: UNIVERSITY OF IOWA
GROUP: T-1
MENTOR: PING YANG
DISCIPLINE: CHEMISTRY
SUBJECT AREA: COMPUTATIONAL CHEMISTRY/ACTINIDE CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26360

INFLUENCING NEPTUNIUM PROPERTIES THROUGH LIGAND FUNCTIONALIZATION

Neptunium makes up the largest percentage of minor actinides found in spent nuclear fuel, but separations of this element have proven difficult due to its diverse redox chemistry. New technologies for minor actinide separations focus on ligands containing either carboxylate or pyridine functional groups, and here, we use first-principles theory to study their interactions with NpO22+/+. Due to their high functionalizability, we systematically tune the electronic properties of the ligands through inclusion of electron-withdrawing and -donating groups. We observe changes in geometric properties, bonding characterization, and NpO22+/+ electronic structure. These properties also impact the Np(VI/V) redox couple, which sheds light on design principles to stabilize different Np oxidation states.

KITMIN CHEN

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF OREGON
GROUP: MST-7
MENTOR: DALI YANG

DISCIPLINE: CHEMISTRY
SUBJECT AREA: MATERIAL AGING AND MASS SPECTROMETRY
TYPE: GROUP PRESENTATION
LA-UR-22-26687

NON-TARGETED IDENTIFICATION OF ANTIOXIDANT DERIVATIVES

Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry Analysis of Eutectic Bis(2,2-dinitropropyl) Acetal/Formal Degradation Profile.

JORDAN EHRMAN

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF WASHINGTON
GROUP: T-1
MENTOR: PING YANG
DISCIPLINE: CHEMISTRY
SUBJECT AREA: THEORETICAL CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27041

THEORETICAL CHEMISTRY

Bonding in actinyl molecules is the focus of ongoing research and debate in the heavy element community and is important for solving challenges in environmental and nuclear science. The participation of the 5f electrons in the covalency of these species is now well-established, but the effect of correlating 6d electrons is less researched. By using computational methods to investigate the role of 6d electrons in the X-ray absorption spectra of actinyl systems, these results will be analyzed to understand the trend of 6d participation in these transitions across the actinide series. These findings will inform the interpretation of actinyl X-ray spectra as they relate to the covalency of the actinide-oxygen bond.

NICHOLAS GARCIA

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF MINNESOTA- TWIN CITIES
GROUP: C-IIAC
MENTOR: JACQUELINE KIPLINGER
DISCIPLINE: CHEMISTRY
SUBJECT AREA: INORGANIC CHEMISTRY/ACTINIDE CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27634

SYNTHESIS, CHARACTERIZATION, AND REACTIVITY OF A NEW CLASS OF URANIUM COMPLEXES SUPPORTED BY NITROGEN/PHOSPHORUS LIGANDS

The chemistry of the actinides has been a growing field over the last few decades due to their relatively unknown nature. While there is a growing number of unique actinide complexes, the field is currently dominated by strong field donating ligands, such as metallocene ligands, or stabilized via multiply bonded species, such as oxo and imido complexes. The employment of phosphino-amide ligand frameworks in actinide compounds have begun to receive attention for the synthesis of heterobimetallic complexes, but the extensive characterization and reactivity of the monometallic actinide complex is limited to date. Herein we report the synthesis and characterization of a triad of uranium phosphino-amide complexes. Additionally, the homoleptic complex U(i Pr2PCH2NPh)4, or U(LNP)4, features unique redox activity and reactivity. An isostructural series of low– and high–valent uranium complexes were successfully isolated, as well as two unique U(VI) complexes.

SARAH GRUNAU

PROGRAM: UNDERGRADUATE
SCHOOL: GEORGE FOX UNIVERSITY
GROUP: MST-7
MENTOR: AMANDA GRAFF
DISCIPLINE: CHEMISTRY
SUBJECT AREA: RADIATION DETECTION MATERIALS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27035

QUANTUM DOTS FOR ENHANCEMENT OF SCINTILLATING RADIATION DETECTION

This project investigates the effects of incorporating semiconductor nanocrystals, or quantum dots (QDs), into scintillating polymer composites with the application of detecting various kinds of radiation. Scintillators are materials that, when struck by high energy photons, such as gamma rays, they emit lower energy photons, usually in the form of visible light. Organic scintillators (often plastics) are easily producible in bulk, are inexpensive and efficient, but are much less accurate in their sensitivity to radiation than inorganic scintillators. The objective of this study is to synthesize and incorporate QDs into the low-cost polymer matrices of organic scintillating materials to improve their overall effectiveness in radiation detection applications.

MIRANDA HILLER

PROGRAM: POST BACHELORS
SCHOOL: UNIVERSITY OF MARY WASHINGTON
GROUP: C-PCS
MENTOR: JESSICA KUBICEK-SUTHERLAND
DISCIPLINE: CHEMISTRY
SUBJECT AREA: MEMBRANE PHYSICAL CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26636

SYNTHETIC HOST-MIMICS FOR SEQUESTRATION OF ENDOTOXIN

Endotoxin, also known as lipopolysaccharide (LPS), is the main molecular cause of sepsis, a severe infection responsible for killing as many as 11 million people per year. Bacteria release LPS into the host bloodstream where it interacts with several host molecules including lipopolysaccharide binding protein (LBP) to initiate a signaling cascade that can lead to sepsis. Our goal is to create synthetic molecules that mimic these host-pathogen interactions to sequester and clear LPS without leading to immune activation. In this work, we have created several synthetic versions of host LPS-binding molecules and measured their binding affinity to LPS using isothermal titration calorimetry (ITC). In the future, these molecules could be used as a therapeutic to delay the onset of sepsis.

CAN LIAO

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF WASHINGTON
GROUP: T-1
MENTOR: JOSEPH KASPER
DISCIPLINE: CHEMISTRY
SUBJECT AREA: ELECTRONIC STRUCTURE THEORY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27211

LOW-SCALING PERTURBATIVE SPIN-ORBIT COUPLING METHOD FOR ACTINIDES

Spin-orbit coupling (SOC) is a cornerstone of modern chemistry that is responsible for numerous phenomena such as fine-structure splitting and intersystem crossing. Modeling SOC has shown to be difficult with available methods being prohibitively expensive for large molecules. A low-scaling method is presented where SOC is included perturbatively to restricted TDDFT by using excitation amplitudes to approximate a wavefunction to form an effective SOC Hamiltonian. The validity of this method will be tested against fine-structure splitting and potential energy surfaces obtained from other theoretical methods and experimental data. This method will be employed to study actinide and transition metal complexes with large ligands where SOC is prominent.

ALEXANDER LIVESCU

PROGRAM: HIGH SCHOOL
SCHOOL: LOS ALAMOS HIGH SCHOOL
GROUP: C-IIAC
MENTOR: XIAOKUN YANG (CLAIRE)

DISCIPLINE: CHEMISTRY
SUBJECT AREA: RENEWABLE ENERGY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26630

BIO-DERIVED DIOXOLANES AS RENEWABLE DIESEL FUEL

Dioxolanes as important intermediates in the production of many value-added chemicals are also showing excellent fuel properties as biodiesel fuel themselves. We report the synthesis and phase separation of two dioxolane compounds from 2,3-BDO via acetalization with two different aldehydes, separately, over heterogeneous catalyst. Fuel properties of the produced compounds were tested and compared with current biodiesel fuels. An accelerated aging and oxidation setup was also applied to the dioxolanes in order to mimic real-world conditions, and the resulting esters were tested for fuel properties to investigate the effects of dioxolane degradation. The fuel properties were observed to change significantly after the aging process, and the compounds were analyzed for biodiesel suitability.

RAVYN MALATESTA

PROGRAM: GRADUATE
SCHOOL: GEORGIA INSTITUTE OF TECHNOLOGY
GROUP: T-4, CNLS
MENTOR: ANDREI PIRYATINSKI
DISCIPLINE: CHEMISTRY
SUBJECT AREA: PHYSICAL CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-25865

PROBING QUANTUM CORRELATIONS IN MOLECULAR SYSTEMS WITH ENTANGLED PHOTONS

Quantum-light is a powerful but mostly untapped tool in the field of molecular spectroscopy. We develop a theoretical framework to treat scattering of quantum photons by open quantum systems and use quantum process tomography to describe the interactions of polarization- entangled biphoton states with molecular systems. Using this theory, we build a computational tool to model spectroscopic signatures of electronic excitations in a complex molecular system, TIPS-tetracene, which undergoes efficient endothermic singlet fission. We simulate spectroscopic signatures of possible singlet fission mechanisms involving quantum correlations, e.g., spin-entanglement of the triplet-triplet pair intermediate in singlet fission, to set the stage for their experimental validations.

NILESH MUKUNDAN

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF CALIFORNIA SAN DIEGO
GROUP: C-NR
MENTOR: JEREMY INGLIS
DISCIPLINE: CHEMISTRY
SUBJECT AREA: NUCLEAR CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27199

NUCLEAR CONTAMINATION IN SEQUENTIALLY GROWN TURTLE SCUTE

Chelonians (turtles, tortoises, etc.) grow scute keratin – the protein structure covering their shells – in sequential layers over time. Here we explore how the scute of chelonians in areas with a legacy of nuclear activity can act as a time-stamped record of radionuclide contamination in the environment. This is significant given that for other chronologically controlled tissues (e.g., tree rings), anthropogenic radionuclides are mobile and appear in years prior to the first deployment of nuclear weapons in 1945. We are analyzing numerous samples from areas of known legacy contamination in order to understand uranium and plutonium contamination. Our results confirm that chelonians can bioaccumulate radionuclides that they are exposed to and do so sequentially over time.

VICTORIA NISOLI

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF NEW MEXICO
GROUP: MPA-CINT
MENTOR: JENNIFER HOLLINGSWORTH
DISCIPLINE: CHEMISTRY
SUBJECT AREA: NANOMATERIALS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27354

NOVEL SPINEL METAL-OXIDE NANOMATERIALS WITH INFRARED PLASMONIC BEHAVIOR

Infrared (IR) plasmonic nanomaterials have utility for enhancing light-matter interactions in applications such as chemical sensing and optical communications. Previously, noble metal and semiconducting chalcogenide plasmonics have been explored, yet they have many shortcomings, particularly in terms of limited ability to shift the plasmonic response to the IR region. A new material system in semiconducting plasmonics—self-doping spinel metal oxides—are shown to support infrared localized surface plasmon resonances (LSPRs) via facile formation of cation antisite defects of metal vacancies. With emphasis on iron and gallium-metal spinel oxides, we demonstrate the ability to synthesize nanocrystals over a broad composition range and the presence of IR LSPRs in many of these.

OSVALDO ORDONEZ

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF CALIFORNIA, SANTA BARBARA
GROUP: C-IIAC
MENTOR: ANDREW GAUNT
DISCIPLINE: CHEMISTRY
SUBJECT AREA: ACTINIDE CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26632

NEPTUNIUM-LIGAND MULTIPLE BONDING

A key fundamental question in actinide chemistry is the extent to which covalency influences the physical and reactivity properties of the 5f elements. Multiple bonds can provide deep insight into metal-ligand valance orbital interactions. This project builds upon developments at the University of California, Santa Barbara in uranium and thorium multiple bonds to nitrogen and carbon donor ligands with the goal of isolating neptunium nitride and allenylidene complexes at LANL. The project takes advantage of specialist radiological facilities at LANL and utilizes recently established neptunium silylamide complexes as synthetic precursors. The results advance comprehension of actinide reactivity and bonding trends as the 5f series in traversed to progressively heavier elements.

BENJAMIN WALUSIAK

PROGRAM: GRADUATE
SCHOOL: GEORGE WASHINGTON UNIVERSITY
GROUP: MST-16
MENTOR: ALICE SMITH
DISCIPLINE: CHEMISTRY
SUBJECT AREA: INORGANIC CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26875

CHARACTERIZATION OF CS2UCL6 AND CS2UO2CL4 FROM ROOM TEMPERATURE TO MELTING

Recently the advantages of molten uranium chloride fuels have been recognized for fast spectrum molten salt reactors (FSMSR's) in particular. Attention should therefore be given to uranium chloride phases that could form as fission in the reactor progresses, or in MSR waste streams. Cesium, being a major fission product, is known to form salts with uranium and uranyl chlorides in the form of Cs2UCl6, and Cs2UO2Cl4 (U4+ and U6+ respectively). Although these compounds are known, their behavior from room temperature to melting has not been completely and unambiguously carried out. Phase transitions, including melting, and crystal lattice changes will be characterized by powder X-ray diffraction, differential scanning calorimetry, and time of flight neutron diffraction.

RIGOBERT YBARRA JR.

PROGRAM: POST BACHELORS
SCHOOL: UNIVERSITY OF TEXAS RIO GRADE VALLEY
GROUP: MPA-11
MENTOR: DANEIL LEONARD
DISCIPLINE: CHEMISTRY
SUBJECT AREA: MATERIALS SYNTHESIS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27158

ENERGY EFFICIENT, HIGH TEMPERATURE CO2 ELECTROLYSIS

CO2 is one of the most common greenhouse gasses contributing to climate change, but carbon is essential for most industrial processes that power society. Due to this, an efficient means of recycling CO2 may help reduce the need for fossil sources of carbon to supply industry. CO2 electrolysis is of significant research interest for the conversion of CO2 to other products, such as CO, COOH. However, significant challenges, like high operating potential and low CO2 reduction efficiency, have hindered development. In order for this technology to be viable, the reduction of CO2 must take place at lower potentials and with higher efficiencies. To achieve these goals we are developing a CO2 electrolysis system that operates at lower cell potential and without aqueous electrolytes.

COMPUTING AND INFORMATION TECHNOLOGY

DAMIAN AXEL BROWNE

PROGRAM: POST BACHELORS
SCHOOL: LOYOLA MARYMOUNT UNIVERSITY

EDGAR JARAMILLO RODRIGUEZ

PROGRAM: PHD SUMMER STUDENT
SCHOOL: UNIVERSITY OF CALIFORNIA DAVIS

GROUP: A-1
MENTOR: GEOFFREY FAIRCHILD

DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: MATHEMATICAL MODELING
TYPE: GROUP PRESENTATION
LA-UR-22-26774

EPISURV: COMMUNITY DETECTION AND SURVEILLANCE FOR AGENT-BASED MODELS

In this paper, we explore the community structure of a massive contact network derived from 'EpiCast,' an agent-based, large-scale model for disease spread. Through an agglomerative hierarchical clustering scheme, we determine the hierarchical community structure of this massive network. We then show how these communities can inform optimal policies for such problems as how to select sensors for early detection and how to allocate vaccines to suppress infections. We also perform exploratory data analysis on these clusters with the goal of revealing common attributes in their members that might further affect policy choices.

HYUNGJIN CHUNG

PROGRAM: GRADUATE
SCHOOL: KOREA ADVANCED INSTITUTE OF SCIENCE AND TECHNOLOGY
GROUP: T-5
MENTOR: MICHAEL MCCANN

DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: MACHINE LEARNING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27727

DIFFUSION MODELS FOR BAYESIAN RECONSTRUCTION IN SPARSE-VIEW X-RAY CT

We will attempt to use diffusion models, which is a trending new class of powerful generative model, in order to develop a 3D reconstruction algorithm for sparse-view X-ray CT. This will be performed without task-specific training and thus in an unsupervised fashion, leveraging the bayesian framework.

SAIKAT DEY

PROGRAM: SUMMER INTERN
SCHOOL: VIRGINIA TECH
GROUP: CCS-3
MENTOR: DIVYA BANESH
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: MATHEMATICS & COMPUTING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27338

FAST GAUSSIAN PROCESS ESTIMATION FOR IN-SITU INFERENCE USING GNN

Exascale computing applications such as climate analysis face significant I/O limitations. A viable solution is to fit statistical models over the data in-situ, that is, inside the simulation as it runs. Gaussian processes (GPs) have state-of-the-art predictive performance for modeling spatial data. Traditional statistical models can calculate GPs hyperparameters accurately, however, they are extremely slow. In the presented work, we use a Graph Neural Network for fast prediction of GP parameters for a spatial dataset. The advantage of using graphs over other models is that graphs can be applied to irregular spatial data. Our preliminary results show that in comparison to the standard methods, our parameter estimates are similar and the predictive performance is orders of magnitude faster.

DESIREE DOMINGUEZ

PROGRAM: UNDERGRADUATE
SCHOOL: FLORIDA INTERNATIONAL UNIVERSITY
GROUP: CCS-3
MENTOR: DIVYA BANESH
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: DATA SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27335

USING NEURAL NETWORKS TO PREDICT DATA VISUALS

As scientists seek to answer domain-related questions, it's common to set up an ensemble of simulations where one or more input parameters are varied to examine how these changes affect the simulation outputs. For large simulations, given limited computing resources, it can be impossible to try every interesting combination of parameters. In this project, we gather feature-based and statistical attributes from simulation results to help scientists better understand how varying input parameters impact results. In addition, we use this ensemble of input parameters to build a machine learning model to help scientists predict outputs between sampled locations of the parameter space. The objective is to determine whether a neural network can reasonably replicate the scientist’s visual outputs.

EMMA DROBINA

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF FLORIDA
GROUP: CCS-3
MENTOR: ELISABETH MOORE

DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: MACHINE LEARNING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26928

EXPLAINABLE MACHINE LEARNING FOR SATELLITE IMAGERY DATA

Many explainable and interpretable machine learning methods have been proposed for image classification neural networks. However, these methods are 1) not statistically verifiable, and 2) largely tested on datasets like CIFAR-10, which are composed of easily human-recognizable objects. We examine methods of statistically quantifying the difference in model understanding across training epochs and explore pitfalls and shortcomings of common image explanation methods when applied to satellite land usage data. Our preliminary results indicate that many image explanation methods are generated in large part from edges within the image, and exclude color- and texture-based features that are important to the model.

GIOVANNI MICHEL

PROGRAM: UNDERGRADUATE
SCHOOL: FLORIDA ATLANTIC UNIVERSITY
GROUP: CCS-3
MENTOR: JESUS PULIDO, TERECE TURTON
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: INFORMATION SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26917

DATABASE VISUALIZATION FOR THE DATA SCIENCE INFRASTRUCTURE PROJECT

The Data Science Infrastructure (DSI) project is focused on providing data management workflows for existing LANL applications such as the Common Model Framework (CMF) via databases (SQL) through defined schema. This approach to data management uses many forms of metadata (simulation, filesystem, performance metrics) to populate a searchable database to enable capabilities for analysis, exploration and visualization. The research efforts in this project involve the exploration of relational and nonrelational databases, deployment in a variety of filesystems on LANL HPC platforms and integration into existing simulation frameworks to automatically cache important metadata. This summer’s research focuses on database visualization (front-ends) interfacing with existing database back-ends.

SONAL JHA

PROGRAM: GRADUATE
SCHOOL: VIRGINIA TECH
GROUP: CCS-3
MENTOR: AYAN BISWAS

DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: ENGINEERING AND MATHEMATICS & COMPUTING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27276

GNN-ASSISTED SAMPLING FOR LARGE-SCALE COSMOLOGICAL SIMULATION

Modern day high-performance computing has enabled large-scale simulations that generate extraordinary amounts of data. However, post hoc analysis of the data is limited by storage and I/O constraints. Sampling has been a popular approach for data downsizing but preserving regions of interest is of prime importance for scientific discovery. We propose a Graph Neural Network (GNN)-assisted sampling method for the Nyx cosmology simulation dataset with a goal of preserving the 'Halos'. Our model provides importance scores to blocks of data based on Halo presence, thereby indicating which blocks are more important for sampling. We evaluate our method by comparing the number of Halos that have been preserved after reconstruction of the sampled output with the number in the original dataset.

RAVINDRA MANGAR

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF COLORADO BOULDER

SAHNI HARSHITA

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF NEW MEXICO

GROUP: XCP-2
MENTOR: CARENE LARMAT
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: HIGH PERFORMANCE COMPUTING & MACHINE LEARNING
TYPE: GROUP PRESENTATION
LA-UR-22-27038

DISCRIMINATING EARTHQUAKES FROM EXPLOSIONS USING HPC AND MACHINE LEARNING

The unique seismic properties of explosions and earthquakes can be used to create a real time signal processing routine that will help to distinguish the two. In this work, we propose a Machine Learning (ML) and High Performance Computing (HPC) pipeline to classify the time series seismic data occurring from earthquakes and explosions in real-time. Another goal of the project is the parallelization of data analysis as well as running some HPC modeling of wave propagation in Rock Valley. We simulated the data using SPECFEM3D. SPECFEM3D is an earthquake simulation software that is optimized for parallel use on a HPC cluster. We employ a 1D Convolutional Neural Network for predicting the two classes in runtime and trained the model on waveforms generated by SPECFEM3D.

MAXIM MORARU

PROGRAM: GUEST STUDENT
SCHOOL: UNIVERSITY OF REIMS CHAMPAGNE-ARDENNE

MINA WARNET

PROGRAM: GUEST STUDENT
SCHOOL: UNIVERSITY OF REIMS CHAMPAGNE-ARDENNE

GROUP: CCS-7
MENTOR: JULIEN LOISEAU
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: COMPUTER SCIENCE
TYPE: GROUP PRESENTATION
LA-UR-22-26750

TEE-ACM

Chain matrix multiplication plays a key role in the training of deep learning models, but also in physics and computer graphics. Matrix multiplications often cause a huge bottleneck in terms of performance and energy, because of the heavy costs in computations and memory operations. Thus, reducing the energetic cost of these types of computation is a major challenge. GPU power consumption is heavily impacted by the number of data transfers performed. In fact, a data transfer from global memory needs one thousand times more energy than a double precision arithmetic operation. Thus, minimizing data transfers is key in reducing energy consumption. Our poster presents an energy efficient solution for Matrix Chain Multiplication on GPUs that minimizes computation and off-chip data transfers.

SHREY POSHIYA

PROGRAM: HIGH SCHOOL
SCHOOL: SANTA FE PREPARATORY SCHOOL
GROUP: CCS-3
MENTOR: DIANE OYEN
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: MACHINE LEARNING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27168

EXPLORING REPRESENTATIONS LEARNED FROM IMAGE TRANSFORMATIONS AS PRETEXT TASKS

Recent advancements in computer vision and deep learning have given rise to models that can learn high-level representations. However, the complexity of these models has resulted in the need for large amounts of labeled data, which is very expensive and time-consuming to obtain. Self-Supervised Representation Learning strives to learn deep features from images without the need for labeled data. Our models are trained to recognize image trans- formations after quantizing the augmentation strength to discrete levels. The resulting representations are then evaluated on their performance on downstream tasks of interest (e.g. linear classification). Our initial results indicate that trying to predict image augmentation strength can lead to learning meaningful representations.

MIRABEL REID

PROGRAM: GRADUATE
SCHOOL: GEORGIA INSTITUTE OF TECHNOLOGY
GROUP: CCS-7
MENTOR: CHRISTINE SWEENEY
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: DATA SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26335

METADATA TRACKING FOR MACHINE LEARNING WORKFLOW

Outside of the simplest models, most machine learning models require many iterations of hyper-parameter tuning, feature engineering, and debugging to produce effective results. As machine learning models become more complicated, this pipeline becomes more difficult to manage effectively. In particular, there is an ever-increasing pool of metadata that is generated by the scientific research cycle. Tracking this metadata can reduce redundant work, improve reproducibility, and aid in the feature and training dataset engineering process. In this project, we investigate a use case for ML metadata management, build a tool to manage the ML pipeline and evaluate the efficacy of this tool against the initial research workflow.

NITEYA SHAH

PROGRAM: GRADUATE
SCHOOL: VIRGINIA TECH
GROUP: CCS-7
MENTOR: CHRISTINE SWEENEY
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: COMPUTATIONAL SCIENCE
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26645

IMPROVEMENTS TO HARDWARE-ACCELERATED 3D SPI DATA RECONSTRUCTION

Fast analysis of scientific data from experimental facilities is key to supporting real-time decisions that efficiently use these facilities and that speed up scientific discovery. Our research shows gains made using graphics processing units (GPUs) to accelerate 3D reconstruction of single particle imaging (SPI) X-ray diffraction data. Reconstructing images of macromolecules is key for innovations in electronics, microbiology, optics, and nanotechnology. We showcase techniques to optimize the per-node computational efficiency and improve the accuracy of SPI by using better algorithms, improving data movement and access, reusing data structures and reducing memory fragmentation. We achieve a 4X speedup and 50% better image reconstruction resolution over the existing GPU implementation.

MICHAEL TETI

PROGRAM: GRADUATE
SCHOOL: FLORIDA ATLANTIC UNIVERSITY
GROUP: A-4
MENTOR: JUSTON MOORE
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: MACHINE LEARNING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26511

LCANETS: LATERAL COMPETITION IMPROVES ROBUSTNESS AGAINST CORRUPTION AND ATTACK

Although Convolutional Neural Networks (CNNs) achieve high accuracy on image recognition tasks, they lack the robustness of biological visual systems. Previous CNNs with frontends modeling the primate visual system exhibited state-of-the-art (SOTA) robustness, but they had limited applicability. Motivated by evidence that neural activity is sparse, we develop a class of CNNs called LCANets, which feature a frontend that performs sparse coding via local lateral competition, and we show that they outperform SOTA CNNs under various corruptions. By performing adversarial attacks on LCANets, we also show that sparse coding CNN layers may not be as robust to white-box attacks as previously thought. Finally, we show that LCA front ends can be used to augment the robustness of current robust CNNs.

DAOCE WANG

PROGRAM: GRADUATE
SCHOOL: WASHINGTON STATE UNIVERSITY
GROUP: CCS-3
MENTOR: JESUS J. PULIDO

DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: HIGH PERFORMANCE COMPUTING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26918

ERROR-BOUNDED LOSSY COMPRESSION FOR 3D AMR SIMULATIONS

The ExaSky Exascale Computing Project (ECP) aims to solve science challenge problems with managing very large cosmological simulations with leading codes HACC and Nyx. One of LANL's roles is to investigate the effects of lossy data compression for massive cosmology simulation datasets. The goal is to evaluate and integrate error-bound lossy compression methods that maximize storage saved on Adaptive Mesh Refined (AMR) data. The challenging aspects of the new approach involve updating and predicting compression parameters as the simulation runs for each time-step and each node cluster, and having the code function efficiently in a highly distributed fashion. The open-sourced code will be implemented into Nyx, where the compute-time, storage, and compression statistics will be measured.

FRANK WANYE

PROGRAM: GRADUATE
SCHOOL: VIRGINIA TECH
GROUP: CCS-3
MENTOR: AYAN BISWAS
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: COMPUTER SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27167

GRAPH-BASED SAMPLING FOR COSMOLOGICAL SIMULATIONS

Scientific simulations generate large amounts of data that need to be saved to disk for further analysis, leading to a burden on I/O systems. There is the need to reduce the amount of I/O performed by these simulations without compromising the quality of generated data. One such simulation is Nyx, which models the spread of dark matter through the universe over time. A common post-hoc analysis in Nyx simulation data is identifying and measuring the size of dark matter halos. In this work, we develop a parallel, adaptive, data-driven graph-based method for sampling from the Nyx simulation data to reduce its I/O footprint. We show that upon reconstruction, our sampling method preserves halo mass more accurately and at smaller sample sizes than current state-of-the-art sampling methods.

STEVEN WILLIAMS

PROGRAM: POST MASTERS
SCHOOL: UNIVERSITY OF NEW MEXICO
GROUP: MST-7
MENTOR: JOSEPH TORRES

DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: DATA MANAGEMENT
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27093

GRANTA IMPORTERS FOR ADDITIVE MANUFACTURING DATA

Granta MI database is incorporated as the central database for material data produced by Additive manufacturing. It is important to capture a multitude of data including project, operator, and build information. Storing data in a centralized location provides access and viewability internally and externally. It also streamlines research and processes necessary to advance the data and perform statistical analysis. AM operators can reference past builds to refine and optimize their builds. The most efficient way to import data from Additive manufacturing is using excel importers. Granta MI has the capability to import and export data directly to and from excel spreadsheet. Granta importers can automate and drastically reduce the time it takes a user to upload large amounts of data records. This work will focus on developing importers to support technology maturation of AM technologies.

EARTH AND SPACE SCIENCES

NEHA AYYALAPU

PROGRAM: UNDERGRADUATE
SCHOOL: PRINCETON UNIVERSITY
GROUP: XTD-IDA
MENTOR: RACHEL SMULLEN
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: THEORETICAL ASTROPHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27198

INSTABILITY PREDICTION IN DIVERSE PLANETARY SYSTEMS WITH MACHINE LEARNING

Machine learning has proven to be an invaluable tool for characterizing the stability of planets in planetary systems. Previously, we investigated the performance of a machine learning classifier on highly diverse planetary systems. In this work, we update our methodology to use a more modern understanding of planetary system architectures. Using information derived from numerical simulations about a planet's early orbital evolution, we train a random forest classifier to predict instability. We explore the predictive power of individual characteristics of planetary orbits towards future instability. The methods like those utilized in this work provide powerful tools to complement numerical simulations across a wide range of planetary architectures.

YAO GAHOUNZO

PROGRAM: GRADUATE
SCHOOL: BOISE STATE UNIVERSITY
GROUP: XCP-2
MENTOR: GIACOMO CAPODAGLIO

DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: OCEAN MODELING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26996

AN IMPROVED B-GRID FORMULATION FOR THE DYNAMICS OF MPAS-SEAICE

B-grid formulations of the sea ice dynamics have been dominant historically because they have matched the grid type used by ocean models. With a B-grid, the sea ice dynamics is solved at the vertices of the mesh cells. The divergence of the stress is the most challenging term to discretize in the sea-ice dynamics, and with a B-grid formulation, each vertex receives contributions from the three cells that share that vertex. For the computation of the divergence of the stress on a spherical mesh, the current formulation of MPAS-Seaice projects the cell coordinates onto planes tangent to the cell centers. We present an alternative approach where the cell coordinates are projected on common planes tangent to the vertex. This approach improves convergence and reduces errors.

SHIRA GOLDHABER-GORDON

PROGRAM: HIGH SCHOOL
SCHOOL: HENRY M. GUNN HIGH SCHOOL

LEXINGTON SMITH

PROGRAM: UNDERGRADUATE
SCHOOL: MACALESTER COLLEGE

GROUP: ISR-6
MENTOR: GRANT MEADORS
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: HELIOPHYSICS
TYPE: GROUP PRESENTATION
LA-UR-22-26661

HELIOSPHERIC DIRECTIONAL SOUNDING: BAYESIAN DISTANCE AND PERIODICITY ESTIMATION

Solar wind (SW) and interstellar medium (ISM) particles exchange charge in the heliosheath (HS), sending energetic neutral atoms (ENAs) back towards the sun. The Interstellar Boundary Explorer (IBEX) satellite measures these ENAs. Reisenfeld et al. (2021) used IBEX data to estimate the distance to the heliosheath using "sounding" across 56 directions: optimal cross-correlations were chosen between time-shifted SW & ENA data based on HS propagation models. Our advance is to use Bayesian inference to sample model parameters and produce uncertainties. We also characterize the frequency spectral ratio of SW and ENA data, searching for any temporal oscillation in HS thickness. These methods can apply to new IBEX maps that separate a "ribbon" feature, and to IMAP after its 2025 launch.

ROWAN JANSENS

PROGRAM: UNDERGRADUATE
SCHOOL: OLIN COLLEGE OF ENGINEERING
GROUP: ISR-2
MENTOR: JAMES WREN
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: ORBITAL MECHANICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27331

IMPROVING SGP4 ORBIT DETERMINATION WITH NEW STATE ESTIMATION ALGORITHM

The Simplified General Perturbations 4 Model (SGP4) is a well-known tool for performing satellite orbit determination. However, uncertainties and inaccuracies in the initial state inputs (required by SGP4) degrade the performance of the propagator. We present a new state estimation algorithm that allows for independent computation of these initial inputs using Unscented Kalman Filtering and GPS data from a satellite. The algorithm is tested on real flight data and demonstrates a notable performance improvement over the standard method of orbit determination using SGP4.

GENEVIEVE KIDMAN

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF NEVADA LAS VEGAS
GROUP: SIGMA 2
MENTOR: DANIEL HOOKS
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: GEOSCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27218

STRESS DISTRIBUTIONS IN POLYCRYSTALLINE QUARTZ USING RAMAN SPECTROSCOPY

The distribution of stress in an elastically anisotropic rock is not well understood, however, the stress distribution is important in how the rock will ultimately deform. I hypothesize that stress percolation describes and explains the heterogeneous stress distribution in a polycrystal that can then lead to shear localization and subsequent deformation. Experimentally measuring stress is possible through Raman spectroscopy which can quantify elastic strain in a crystal lattice between a loaded and non-loaded state. A stress map was created from the pressure dependent 464 cm-1 peak in single crystal and polycrystalline Tigers' Eye quartz. Early results suggest intergranular heterogeneous stress distributions between the grains in the polycrystal that resemble stress percolation patterning.

DOLAN LUCERO

PROGRAM: GRADUATE
SCHOOL: NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY
GROUP: EES-16
MENTOR: SUZANNE BOURRET, PHILIP STAUFFER

DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: EARTH SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27064

RADIONUCLIDE WASTE SIMULATIONS TO ASSESS THE VIABILITY OF SUBSURFACE STORAGE

As part of a collaboration between the U.S. National Nuclear Security Administration (NNSA) and the Israel Atomic Energy Commission (IAEC), we are investigating the viability of subsurface nuclear waste disposal in the Negev Desert, Israel. We present flow and transport simulation results on the effect of heat generating nuclear waste in a proposed intermediate depth borehole located between depths of 150-300 m in the vadose zone. Thermal loading caused by radioactive decay leads to changes in saturation driven by water vapor transport and phase changes. To assess the time- and temperature-dependent changes in proximity to the borehole, we developed a thermal loading model using the Los Alamos multiphase porous flow and transport simulator FEHM.

NOAH MARTIN

PROGRAM: UNDERGRADUATE
SCHOOL: PURDUE UNIVERSITY
GROUP: ISR-3
MENTOR: AMANDA SHERIDAN
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: PLANETARY SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26680

GEOLOGY ON MARS WITH THE SUPERCAM MICROPHONE

Solar wind (SW) and interstellar medium (ISM) particles exchange charge in the heliosheath (HS), sending energetic neutral atoms (ENAs) back towards the sun. The Interstellar Boundary Explorer (IBEX) satellite measures these ENAs. Reisenfeld et al. (2021) used IBEX data to estimate the distance to the heliosheath using "sounding" across 56 directions: optimal cross-correlations were chosen between time-shifted SW & ENA data based on HS propagation models. Our advance is to use Bayesian inference to sample model parameters and produce uncertainties. We also characterize the frequency spectral ratio of SW and ENA data, searching for any temporal oscillation in HS thickness. These methods can apply to new IBEX maps that separate a "ribbon" feature, and to IMAP after its 2025 launch.

MAZEN NAKAD

PROGRAM: GRADUATE
SCHOOL: DUKE UNIVERSITY
GROUP: EES-14
MENTOR: SANNA SEVANTO

DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: ENVIRONMENTAL SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-25983

ECOSYSTEM FUNCTIONAL SIGNATURES FOR REMOTE PROLIFERATION DETECTION

Monitoring nuclear facility operations for treaty compliance is primarily done through either local chemical release sampling or remote satellite and aircraft data acquisition. However, these methods provide data with limited time resolution, are labor-intensive and frequently obvious to the party under investigation. The work presented here explores a new approach for remote nuclear proliferation detection using publicly available data from a global ecosystem monitoring network called Fluxnet. Fluxnet is a physics-based sensor network that continuously measures material and energy fluxes from ecosystems at a high temporal resolution. Using this approach, our focus will be on studying ecosystem response to nuclear facility operation or material releases.

SIOBHAN NIKLASSON

PROGRAM: GRADUATE
SCHOOL: NEW MEXICO TECH UNIVERSITY
GROUP: EES-17
MENTOR: CHARLOTTE ROWE
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: GEOPHYSICS
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-24372

HYDROACOUSTIC MODELING IN A RAPIDLY-EVOLVING ARCTIC

The Arctic Ocean is rapidly warming. This will lead to obsolescence for today's ocean acoustic models. At LANL, we are creating the first version of the Department of Energy's Energy Exascale Earth System Model (E3SM), capable of driving an acoustics model in a rapidly-evolving Arctic Ocean. We analyze E3SM simulations to investigate how well we currently capture water properties of the Arctic water column. We present preliminary results of model validation against temperature and salinity observations. The goal of this effort is to provide boundary conditions to the acoustic model, to enable quantification of the ocean acoustic implications of climate change as well as create a climate-aware atlas of global acoustic noise and propagation adjustments for non-proliferation signal detection.

DULCIE QUINN

PROGRAM: HIGH SCHOOL
SCHOOL: SANTA FE HIGH SCHOOL
GROUP: T-5
MENTOR: PEDRO RESENDIZ LIRA
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: PLASMA PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27190

PROPERTIES OF COLD ELECTRONS IN THE EARTH'S MAGNETOSPHERE

The cold (<100 eV) electrons and ions of the Earth's magnetosphere are poorly measured and understood. Still, they play a key role in the Earth's magnetosphere, impacting critical aspects of the system. Using Python to gather, calculate and plot data (from the Van Allen Probes spacecraft), decomposed into electron populations of different energies, we can analyze the cold electron density and temperature within the magnetosphere as a function of different conditions (time of year, magnetic local time, geomagnetic activity), showing the results as polar scatter and histogram plots. Checks are in place to reduce photoelectron contamination of the results. This is a first step to understanding the cold electrons in the magnetosphere, and the magnetosphere overall.

CAMILLE RENAUD

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF COLORADO, BOULDER
GROUP: XCP-2
MENTOR: CAROLYN BEGEMAN

DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: EARTH SYSTEM MODELING, MACHINE LEARNING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27252

ENABLING SMARTSIM IN MPAS-OCEAN FOR ONLINE MACHINE LEARNING AND DATA ANALYSIS

A formidable challenge in earth system modeling (ESM) is representing processes over a wide range of scales, from global circulation down to 10 km-wide eddies. With today's access to vast quantities of data, machine learning (ML) has the potential to significantly improve parameterizations of these processes for enhanced prediction. However, leveraging ML in ESM has been slow due to inefficient coupling between ESMs, typically written in Fortran/C++, and rapidly evolving ML libraries, typically written in Python. We implement the novel framework SmartSim in E3SM's ocean component MPAS-O which enables the online execution of ML models and simultaneous data exchange. We then demonstrate ML prediction and visualization at simulation runtime and compare offline and online learning results.

JUAN SANCHEZ

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF CENTRAL FLORIDA
GROUP: XCP-2
MENTOR: GOPINATH SANTHANA GANAPATHY SUBRAMANAIAN

DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: COMPUTATIONAL EARTH SCIENCES
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26549

IMPLEMENTATION AND TESTING OF A MATERIAL STRENGTH MODEL FOR GEOLOGICAL MATERIALS

Motivated by the need to improve the capability to monitor potential evasive nuclear explosive tests through scientific research, this project models the effects of the underground detonation of a conventional High Explosive (HE). The subsurface material (tuff) will be modeled using the Schwer-Murray strength model as implemented in a standard hydrodynamics code. Results would include calculations of various metrics of interest, such as size of the cavity produced, wave speed, and other metrics of interest to the project.

KATHERINE SWAGER

PROGRAM: POST MASTERS
GROUP: EES-16
MENTOR: SUZANNE BOURRET
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: HYDROGEOLOGY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27065

3-D URANIUM FATE AND TRANSPORT MODELING IN THE NORTHEASTERN NEGEV DESERT, ISRAEL

To assess the suitability of a site for subsurface radioactive waste disposal in the Negev Desert, Israel, we created a 3-D probabilistic flow and transport model informed by rock properties and uranium sorption characteristics. All samples exhibit intermediate to high sorption capacities suggesting a natural barrier to radionuclide migration. We simulate a scenario where 1000 moles of uranium migrate from the disposal borehole under different infiltration conditions that represent present day and future climate scenarios. Results show the uranium will escape the domain: (1) in over 1000 years under a moderate infiltration flux (30 mm/y); (2) in ~200 years for extreme precipitation conditions (210 mm/y); and (3) in 700 years for a surface ponding scenario, but at low concentrations.

ALLEN TING

PROGRAM: UNDERGRADUATE
SCHOOL: THE UNIVERSITY OF TEXAS AT AUSTIN
GROUP: EES-14
MENTOR: ERIC GUILTINAN
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: CHEMICAL EARTH AND LIFE SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27169

FORECASTING MULTIPHASE FLOW THROUGH FRACTURES WITH CONVOLUTIONAL NEURAL NETWORKS

Fractures are ubiquitous in the subsurface and serve as preferential channels for flow and transport. However, our understanding of the multiphase flow of immiscible liquids in fractured media is still limited, partially due to the computational challenges of running expensive physics-based simulations. In this project, we utilize physics-constrained convolutional neural networks and state-of-the-art computer vision techniques to forecast the state of liquid carbon dioxide in a fracture through time. We also propose a workflow to generate 2D representations of 3D simulation data to uniquely describe the fluids within a fracture. The results will have implications in application spaces including oil and gas production, geothermal energy, CO2 sequestration, and nuclear waste disposal.

SABRINA VOLPONI

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF NOTRE DAME
GROUP: EES-16
MENTOR: JEFFREY HYMAN
DISCIPLINE: EARTH AND SPACE SCIENCES
SUBJECT AREA: GEOSCIENCES
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26949

THE ROLE OF FINITE BLOCK SIZE MATRIX DIFFUSION ON TRANSPORT IN FRACTURED MEDIA

Modeling particle transport within subsurface fractures is critical to national security issues, such as nuclear waste disposal. Breakthrough curve shape, in this context, is influenced by mass transfer between the fracture network and the surrounding rock matrix. Previous work studied this interplay assuming infinite matrix block size, neglecting the potential of a particle transferring into nearby fractures and over estimating transport time. In this study, we assess the impact of finite matrix block size on breakthrough curve profiles at different spatiotemporal scales. Breakthrough curves are generated using particle tracking simulations within the three-dimensional discrete fracture network simulator dfnWorks, where matrix diffusion is integrated using a time-domain random walk.

ENGINEERING
(ALL DISCIPLINES)

THOMAS ALLARD

PROGRAM: GFSD-FELLOW
SCHOOL: CU BOULDER
GROUP: W-13
MENTOR: NATHAN MILLER
DISCIPLINE: ENGINEERING
SUBJECT AREA: CIVIL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27205

TARDIGRADE MICROMORPHIC SOFTWARE PACKAGE FOR SIMULATION OF A BONDED MATERIAL

Predicting the mechanical response and failure of heterogenous materials has proven difficult. Multiscale numerical methods based in higher order continuum theories attempt to bridge the gap between micro- and macro-structural behavior. Micromorphic continuum theories have shown promise. The Tardigrade software package is an implantation of Eringen's micromorphic continuum theory that leverages the finite element (FE) framework of Idaho National Laboratory's MOOSE software. This work investigates Tardigrade's ability to capture the response of a bonded particulate material. Direct numerical simulations results are processed using Tardigrade's micromorphic filter, a material model is calibrated, and micrormophic simulation are performed.

ERICK ALVAREZ VELAZQUEZ

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF TEXAS AT EL PASO
GROUP: ALDWP-TAO
MENTOR: MICHAEL FERRY

NATHAN KWAKU OPOKU SAPONG

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF SOUTHERN CALIFORNIA
GROUP: E-1
MENTOR: MIKE FLORES

DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR MATERIAL CONTROL AND ACCOUNTABILITY
TYPE: GROUP PRESENTATION
LA-UR-22-26940

EXPERIMENTATION AND DATA ANALYSIS FOR RADIO FREQUENCY TAG IDENTIFICATION

Radio Frequency Identification (RFID) technology has been identified as a promising solution to reduce inventory management workload at increasing production levels across the NNSA/DOE complex. RFID has the potential to enable faster active inventory ID, improved daily administrative checks and plant alignment verification. This project aims to evaluate the effectiveness of RFID devices and tags for inventory management. Using a two-level shelf layout, test parameters such as reader motion, distance, and power level are varied over thousands of tests using a handheld RFID scanner and 50 tags attached to container exteriors. Statistical analysis is performed to evaluate data trends and determine efficient RFID device usages for operators.

ISAIAH ARCHULETA

PROGRAM: UNDERGRADUATE
SCHOOL: NEW MEXICO STATE UNIVERSITY
GROUP: IQPA-MPCL
MENTOR: MATTHEW SCHROLD
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27163

CALIBRATION OF ACCELEROMETERS USING A TEMPERATURE CONTROLLED ENVIRONMENT

The main goal of the project was to complete a bench operability checklist for a SPEKTRA temperature Test Calibration System. This involved coming up with an uncertainty budget and calibration procedure for the test system which are important steps in helping the machine get closer to being used in the cal. lab. Also before being able to work on the main goals for the SPEKTRA, I had to first learn how to calibrate accelerometers using the calibration systems currently used in the calibration lab which was also to help me better understand how the systems and accelerometers themselves work. Overall we came up with a rough draft for both the budget and procedure.

CODY BAKER

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS TECH UNIVERSITY
GROUP: AOT-RFE
MENTOR: SUNG II KWON
DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27225

MODELING AND SIMULATION OF ELECTRIC FIELDS IN RF CAVITIES

This project focuses on computational modeling of electric fields in 805 MHz resonance cavities. A state-space representation of an RF cavity was converted into a Simulink model to allow simulation. This model depends on measured physical quantities of the cavity to parameterize the model. A graphical user interface (GUI) was also made to make changing model parameters easier. Data collection was done for 805 MHz RF cavities to provide input for the model. Time constant determination was automated for each cavity to increase model accuracy. Transient and frequency response of each cavity of the Linac were obtained via simulation. A stochastic model was also written to learn system dynamics using input cavity field data using a neural network.

SARBAJIT BASU

PROGRAM: GRADUATE
SCHOOL: NEW MEXICO STATE UNIVERSITY
GROUP: A-1
MENTOR: ARTHUR BARNES, ADAM MATE

DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27074

DYNAMIC STATE ESTIMATION-BASED PROTECTION FOR INDUCTION MOTOR LOADS

Protective device coordination is critical to maintain the resilience of large microgrids. Inverter-interfaced generation, however, poses significant challenges when designing protection systems. Traditional time-overcurrent protective devices are unsuitable on account of the lack of fault current. Dynamic state estimation (DSE) has been proposed for line protection, and more recently for the protection of load buses or downstream radial portions of microgrids. Passive loads are often considered for modelling and implementation of adaptive protection systems, but dynamic loads such as induction motors behave differently under faulted conditions. This project demonstrates using DSE for adaptive protection in a three-phase induction motor under normal operation and under faulted conditions.

BRANDON BOHANON

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF NEW MEXICO
GROUP: MST-8
MENTOR: ARJEN VEELEN
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27362

DEFECT STRUCTURE OF UO2-BASED ACCIDENT TOLERANT FUELS STUDIED USING XAS

X-ray Absorption Spectroscopy (XAS) is an area of growing interest in the advanced characterization of accident tolerant nuclear fuels. XAS is a sensitive technique that can identify subtle changes in interatomic distances and, therefore, is useful in the identification of structural defects. Moreover, XAS can be used to identify the chemistry of dopants/impurities and determine the possible mechanism of incorporation into the host phase. In this study, we used XAS at the Stanford Synchrotron Radiation Lightsource (SSRL) to investigate the impacts of chromium on the UO2 structure and the effects of sintering conditions on the speciation of chromium. In this presentation we will show the impact of sintering conditions and dopant concentration on UO2 and chromium molecular structures.

MYLES BRADLEY

PROGRAM: UNDERGRADUATE
SCHOOL: UTAH STATE UNIVERSITY
GROUP: AOT-AE
MENTOR: LEANNE DUFFY
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-25924

CERAMIC ENHANCED ACCELERATOR CAVITY SPACE READINESS

An experimental design for a radiofrequency particle accelerator cavity uses a ceramic insert instead of metal conventionally used to form a microwave cavity. Constructing the cavity in this manner results in a power efficiency greater than that found in accelerators of a conventional design. A major drawback of the ceramic accelerator design is that the ceramic is significantly less durable than its conventional metal counterpart. In order to prepare this accelerator design for space flight this project increases the thickness of the ceramic ring in order to improve its structural strength. The electromagnetic modeling program CST is used to model the ceramic insert to determine dimensions that have desirable properties without having to construct and test numerous different models.

JUAN BRANCH

PROGRAM: UNDERGRADUATE
SCHOOL: NEW MEXICO STATE UNIVERSITY
GROUP: ES-IPD
MENTOR: FORREST BLACKBURN
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27227

LANL HVAC AND BAS SYSTEMS OVERVIEW

My project will be discussing the overview and changes that are coming to the LANL HVAC and BAS systems. I will be breaking it down into three pieces. Where we are at right now with our systems. What we want to with these systems (upgrade them). Finally, how will we reach our goal.

NATHANAEL BREED

PROGRAM: UNDERGRADUATE
SCHOOL: LIBERTY UNIVERSITY

VANESSA KALENITS

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF NEVADA RENO

GROUP: J-NV
MENTOR: STEVEN PEMBERTON
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: GROUP PRESENTATION
LA-UR-22-27088

ACOUSTIC ANALYSIS AND CAMERA REMOTE FOCUS SYSTEMS

Over the course of this summer, a method for acoustic analysis was developed with the goal of collecting pressure data in a minimally involved manner. The software behind the GUI works by continuously monitoring the acoustic properties in its vicinity for any events that cross the event threshold which is set by the user in the GUI. The second goal was to develop a system to remotely adjust the focus and zoom of the lenses from an Armag positioned a mile away from the firing point. This was accomplished by programming an Arduino to control a stepper motor which rotated the zoom and focus knobs of the lens using a pulley system. Custom 3D printed mounts were also designed using CAD software (Blender) to attach the motors to the camera lens.

PAPRAPEE BUASON

PROGRAM: GRADUATE
SCHOOL: GEORGIA INSTITUTE OF TECHNOLOGY
GROUP: T-5
MENTOR: SIDHANT MISRA
DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27022

A DATA-DRIVEN METHOD TO IDENTIFY CRITICAL LOCATIONS IN DISTRIBUTION GRIDS

This project studies the sensor placement problem which identifies the locations for installing sensors that can capture all possible voltage violations due to load variability and fluctuation of distributed energy resources in distribution grids. We formulate a bilevel optimization problem that minimizes the number of sensors and avoids false sensor alarms in the upper level while ensuring detection of any violations in the lower level. We develop conservative linear approximations of the power flow equations and problem reformulations, which improve computational tractability while simultaneously ensuring an appropriate placement of sensors.

OLIVIA CANTRELL

PROGRAM: UNDERGRADUATE
SCHOOL: NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY
GROUP: ISR-1
MENTOR: ERNST ESCH (SHORTY)

DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27256

LIGHT DETECTION AND RANGING AT THE TRANSURANIC WASTE FACILITY

The ADReSS Project is in need of accurate "as built" dimensions of the Transuranic Waste Facility (TWF). We used Light Detection and Ranging (LiDAR) to effectively analyze the dimensions of the facility without interfering with the facility content. LiDAR is a process used to calculate the ranges and sizes of various objects and landscapes. The data collected from multiple reflections compose a three-dimensional model called a point cloud. From the point cloud, we composed a SolidWorks model which can be used to eliminate discrepancies between the engineering drawings and reality. This poster describes how a LiDAR system works, how it was used to gather data from the TWF, and how it was used to construct a SolidWorks model.

MIGUEL CHACON CUESTA

PROGRAM: UNDERGRADUATE
SCHOOL: ARIZONA STATE UNIVERSITY
GROUP: P-4
MENTOR: VINCENT GARCIA

DISCIPLINE: ENGINEERING
SUBJECT AREA: ROBOTICS ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27010

PROTOTYPE ROBOTICS ALIGNMENT SYSTEM FOR PHELIX

The objective of this project is to design a prototype robotics alignment system for PHELIX. The goal for this phase of the project is to define the design requirements for the system, determine the software and hardware specifications, and finally select the hardware components needed for the alignment system with a bill of materials. If given enough time, simulating the robotics and creating a 3D scaled model demonstrating that the robotics work will be included in this phase of the project. Finally, the project will be presented in a "design review" environment to gain feedback on the developed requirements and the conceptual design. The deliverables are to create a LANL Student Symposium poster, a Division/Group presentation, internal report(s), and product development.

DEEPANJALI CHOWDHURY

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS A&M UNIVERSITY
GROUP: ISR-4
MENTOR: QUINN COLE
DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: INDIVIDUAL
LA-UR-22-25915

A NOVEL BACKPLANE: COMMUNICATIONS INTERFACE FOR SPACE APPLICATIONS

Space hardware must be capable of reliable, robust data communications. To do so, many space systems rely on printed circuit boards (PCBs) called backplanes to provide the electrical connections through wires and connectors among plug-in modules, which are also typically PCBs. Circuit boards use backplanes to communicate with each other by leveraging system specifications, such as OpenVPX and SpaceVPX. With VPX specifications, the hardware can handle higher mechanical stress and support a wide range of module types and power profiles. This project develops a custom backplane that uses VPX specifications to maintain interoperability with commercial testing hardware along with reducing the cost of the system by eliminating duplicate modules. The goal of this project is to create an interface vital for power distribution and improve space-flight circuit-board communication while minimizing size, weight, and power (SWaP).

JESSICA COOKE

PROGRAM: UNDERGRADUATE
SCHOOL: NEW MEXICO TECH
GROUP: P-2
MENTOR: ERNST ESCH (SHORTY)
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR WASTE HANDELING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27215

ADJUSTABLE CENTER OF GRAVITY LIFT FIXTURE RECONFIGURATION APPARATUS

The aim of the Adjustable Center of Gravity Lift Fixture Reconfiguration Apparatus is to reduce ergonomic injuries, provide a safe workspace for the operators, and compactly store components of the Adjustable Center of Gravity Lift Fixture, a lifting tool made for loading radioactive waste drums into trucks.

THOMAS DEGUIRE

PROGRAM: GRADUATE
SCHOOL: TEXAS A&M UNIVERSITY
GROUP: NEN-1
MENTOR: TOM STOCKMAN
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26566

AN INTEGRATED APPROACH TO PRECISION NEUTRON MEASUREMENTS IN DYNAMIC ENVIRONMENTS

To control background, nuclear material is often transported from a working area into a shielded measurement area. While effective, material movement represents a significant contamination and exposure risk to operators This work aims to remove that step from the process and enable the use of high precision instruments in a dynamic environment. A methodology is demonstrated which uses dispersed neutron detectors in a mock glovebox environment to quantify a dynamic background count rate and remove it from an HLNC measurement. The effectiveness of this methodology is quantified experimentally by measuring the mass of a Cf-252 source in an environment where several other sources are moving throughout the room during the measurement.

ISHA DOGRA

PROGRAM: GRADUATE
SCHOOL: GEORGIA INSTITUTE OF TECHNOLOGY
GROUP: UI-OSI
MENTOR: GENNA WALDVOGEL

DISCIPLINE: ENGINEERING
SUBJECT AREA: ENVIRONMENTAL AND CHEMICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27324

WATER IN COOLING TOWERS: METSICLOPS

The Strategic Computing Complex cooling towers (SCC CTs) provide efficient evaporative cooling using 38 million gallons per year (MGY) of water, with this value projected to peak to 97 MG in FY31 for the proposed Future Supercomputing Infrastructure (FSI). With the current Sanitary Effluent Reclamation Facility (SERF) capacity at 70 MGY, LANL needs sustainable ways to meet that demand. This project investigates both expansion of the SERF treatment system, and less water intensive alternatives to evaporative CTs. Another major water consumer are the Neutron Science Center (LANSCE) CTs that use the County's high Silica-content potable water, which limits the potential for water reuse. This project also studies more clean sources to reduce overall water consumption at LANSCE.

NADEZDA DRAGANIC

PROGRAM: HIGH SCHOOL
SCHOOL: LOS ALAMOS HIGH SCHOOL

JACK AMMERMAN

PROGRAM: HIGH SCHOOL
SCHOOL: LOS ALAMOS HIGH SCHOOL

GROUP: AOT-MDE
MENTOR: BHAVINI SINGH

DISCIPLINE: ENGINEERING
SUBJECT AREA: MODEL-DRIVEN ENGINEERING
TYPE: GROUP PRESENTATION
LA-UR-22-26794

FLOW VISUALIZATION AND ANALYSIS FOR FLOW THROUGH A PIPE WITH VARYING REYNOLD'S NUMBERS

This work explores fluid flow through a pipe with the focus of understanding laminar and turbulent fluid flows. The fluid mechanics of Newtonian fluids were calculated using an understanding of Bernoulli's equation, Reynold's number, and pressure drop in pipe flow. The analytical calculations were then applied to a bench-top experiment where the flow of water in a pre-designed system was studied, and variables like velocity and pipe diameter were modified. MATLAB programs and additional calculations were used to assist in data collection and analysis to determine overall results and conclusions.

SEAN DREWRY

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF TENNESSEE KNOXVILLE
GROUP: MST-8
MENTOR: SCARLETT WIDGEON

DISCIPLINE: ENGINEERING
SUBJECT AREA: MATERIALS SCIENCE- AND ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26806

ENHANCED CHROMIUM DOPED UO2 FUEL FOR LIGHT WATER REACTOR APPLICATIONS

In an effort to design accident tolerant fuels for light water reactors (LWRs), UO_2 has been doped with different additives such as chromium to increase average grain size and density of sintered pellets. These features promote the retention of fission products within the grains and increase plasticity of the fuel pellet. UO_2 powder feedstocks with varying Cr_2O_3 concentrations (ranging from 950 to 7800 ppm) will be sintered. Density of the sintered pellets will be measured, and average grain size will be determined using Scanning Electron Microscopy (SEM) on polished samples. X-ray diffraction will be conducted, and lattice parameter will be determined using Rietveld refinement. Lattice parameter and grain size evolution will be compared as a function of dopant concentration.

MICKY DZUR

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS A&M UNIVERSITY
GROUP: XCP-3
MENTOR: JERAWAN ARMSTRONG
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26149

CUBIT FOR MCNP UNSTRUCTURED MESH ANALYSIS OF OKTAVIAN BENCHMARKS

MCNP6 has the ability to track particles on unstructured mesh (UM) embedded within constructive solid geometry (CSG) cells; an advancement enabling detailed analysis on complex geometry models. A UM geometry model is created by decomposing a solid geometry into finite elements. While there are several programs that can generate UM models for MCNP simulations, this work uses CUBIT to create solid geometries and generate linear hexahedral element models of the Oktavian benchmark experiments. The goal of this work is to verify the MCNP tracking method on linear hexahedron models by comparing results with simulations that use CSG and linear tetrahedron UM models.

JACK FLETCHER

PROGRAM: GRADUATE
SCHOOL: MASSACHUSETTS INSTITUTE OF TECHNOLOGY
GROUP: NEN-2
MENTOR: NICHOLAS THOMPSON
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26440

TOWARDS A BENCHMARK WITH THE COMPACT NUCLEAR POWER SOURCE

The Compact Nuclear Power Source (CNPS) was a high-assay low-enriched uranium tristructural isotropic-fueled, graphite-moderated microreactor built in 1987 at TA-18. In its day, critical experiments with a mock-up of the reactor meaningfully advanced the body of critical and integral data until its disassembly in 1991. This work aims to develop a benchmark based on the CNPS experiment due to interest in similar contemporary microreactors. Uncertainties remain, however, in parameters of the reactor as described in literature and implemented in current computational models. The assessment and minimization of these uncertainties is a crucial step towards a benchmark. This work seeks to initiate this process with a survey of available documentation and refinements to CNPS neutronics models.

MATTHEW GOMEZ

PROGRAM: HIGH SCHOOL
SCHOOL: POJOAQUE VALLEY HIGH SCHOOL

ATHENA GRACE MARTINEZ

PROGRAM: HIGH SCHOOL
SCHOOL: ESPANOLA VALLEY HIGH SCHOOL

GROUP: AOT-RFE
MENTOR: HENRY GAUS III
DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: GROUP PRESENTATION
LA-UR-22-27194

TEMPERATURE CONTROLLER FOR PO1 WATER SYSTEM

Water temperature controller for the LANSCE proton storage ring.

SHAYNA GOMEZ

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS TECH UNIVERSITY
GROUP: AOT-RFE
MENTOR: MARIA SANCHEZ BARRUETA
DISCIPLINE: ENGINEERING
SUBJECT AREA: COMPUTER SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-25268

RADIO FREQUENCY POWER DETECTORS

The Radio Frequency (RF) Power detector is used to perform pulsed RF power measurements of input and output signals for the different amplifier stages feeding the LANSCE DTL (Drift Tube Linac). The power detector needs to be programmed and calibrated to account for differences between devices and to accurately represent all power stages of the amplifiers. Since 2015 the program in this device has been largely unchanged and it now relies on outdated systems to keep it running. Updates to the program have been made to expand on its original capabilities and allow for continued operation and production of these devices. The concentration in this poster is the programming aspect.

ALICIA GONZALES

PROGRAM: UNDERGRADUATE
SCHOOL: NEW MEXICO STATE UNIVERSITY
GROUP: MPA-11
MENTOR: TOMMY ROCKWARD, CORTNEY KRELLER

DISCIPLINE: ENGINEERING
SUBJECT AREA: MATERIALS ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27262

COMPARISON OF GAS DIFFUSION ELECTRODES (GDE) IN AND OPERATING FUEL CELL STACK

Fuel cells are electrochemical devices that combine H2 and O2 to produce clean, efficient energy (electricity). One major component of a fuel cell system is the gas diffusion electrode. GDEs are catalyzed gas diffusion media with multiple functions. They uniformly distribute fuel and react in an operating stack, manage water, and facilitate electrochemical reactions. These reactions govern fuel cell output, require a delicate balance between the reactant gas, Pt catalyst, and proton conducting ionomer referred to as the triple phase interface. This research compares the performance of 8-cell micro fuel cell stacks using various GDEs. The GDEs are from two different suppliers versus LANL GDEs. Tests were run at 25°C using H2 and O2. Initial results show LANL GDEs with the best performance.

ETHAN GRANUCCI

PROGRAM: UNDERGRADUATE
SCHOOL: UTAH VALLEY UNIVERSITY
GROUP: AOT-RFE
MENTOR: PHILLIP TORREZ
DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27248

VALIDATING EFFECTIVE POWER TO RF CAVITY THROUGH MODELING AND MEASUREMENTS

The LANSCE LLRF team is responsible for providing an ultra-fast feedback and feedforward system that maintains the accelerator cavity fields to typically 0.1% and 0.1˚ error, provides a phase stable reference to the accelerator, and interfaces to high power RF systems. The RF drive power can be as high as 1.2 MW, so obtaining a ~10 mW sample of the cavity field requires several stages of coupling, attenuation, and filtering. Similarly, driving the cavity back to 1.2 MW requires filtering and amplification. In this project, the RF signal transmission between the cavity and Feedback Control Module (FCM) is modeled, therefore obtaining a better understanding of how much effective power can be delivered to the cavities. Data for this model was obtained from field data and analytical methods.

COOPER GUILLAUME

PROGRAM: UNDERGRADUATE
SCHOOL: LIBERTY UNIVERSITY
GROUP: J-6
MENTOR: JOSE MARTIN TACCETTI
DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26453

EFFECT ON FOCUSING SOLENOID FIELDS BY FERROMAGNETIC CORES IN LIA CELLS

This project studies the effect of crosstalk between magnetic fields due to saturation effects in ferromagnetic materials used in the DARHT Axis II linear induction accelerator, LIA, cells. Simulation and theoretical calculations are performed to verify the effect. Finally, an experiment was conducted to measure and analyze data to quantify the effect of the saturation on the focusing magnetic field.

MATTHEW HAMMOND

PROGRAM: GRADUATE
SCHOOL: TEXAS A&M UNIVERSITY
GROUP: E-3
MENTOR: BETH BOARDMAN

DISCIPLINE: ENGINEERING
SUBJECT AREA: ROBOTICS AND AUTOMATION
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26620

ROBOTIC RECYCLABLE WASTE SORTING SYSTEM

The Robotic Recyclable Waste Sorting System is part of the effort to reduce the amount of non-recyclable waste generated here at LANL. The system consists of a robotic manipulator coupled with an array of sensors and computer vision program that allow it to identify the material of a given piece of waste and sort it into various bins for easy recycling. It also removes the human element from this undesirable and potentially hazardous task, reducing exposure to chemicals, pathogens, and harmful waste. The RRWSS also serves as a proof of concept for other sorting systems and could be easily adapted to evaluate and decontaminate radioactive materials within a glovebox, ensuring that operators and technicians are not exposed to any harmful levels of radiation.

ALEXANDER HAUCK

PROGRAM: GRADUATE
SCHOOL: THE PENNSYLVANIA STATE UNIVERSITY
GROUP: NEN-2
MENTOR: TRAVIS GROVE
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26825

GENERATING MODELS OF THE FLATTOP CRITICAL ASSEMBLY FOR BENCHMARK EXPERIMENTS WITH PYTHON

Supporting the mission of nuclear criticality safety, the Flattop-HEU benchmark critical experiment is undergoing reevaluation. The reevaluation efforts include precise measurements of the assembly to increase modeling accuracy. This work utilizes Python to efficiently generate MCNP input files for various Flattop configurations based upon the high-fidelity model, starting with the configuration in Flattop-HEU. Python allows for the initial focus to be placed on accurate modeling while subsequent model generation will allow users to "insert" specific components or update values. The code will then adjust the generated input file quickly and meticulously.

MACKENZIE JAMES

PROGRAM: POST BACHELORS
GROUP: ISR-3
MENTOR: BRETT NADLER
DISCIPLINE: ENGINEERING
SUBJECT AREA: COMPUTER SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27330

ADAPTIVE TOOL SETS IN PYTHON FOR MANAGEMENT DECISION MAKING

This set of python tools was created to assist in utilizing discrete Microstrategies (financial) and Primavera 6 (scheduling) data imports for project decision making. These toolsets were built into a user-friendly web app and are also accessible through python IDEs. One of the main objectives of the scheduling toolset is to compare the amount of project effort (i.e. labor) to what had been initially baselined. The corresponding objective for the financial tools is to compare the project costs to what had been forecasted for labor and procurements. Both have plotting and tabular capabilities that summarize calculations and analysis. This project has been focused on the ISR division SABRS space-based payload project, but with further development can be utilized by other projects at the lab.

EVAN JIMENEZ

PROGRAM: UNDERGRADUATE
SCHOOL: NEW MEXICO STATE UNIVERSITY

RUBY MELENDEZ CAMACHO

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS A&M UNIVERSITY

JOSEPH WATKINS

PROGRAM: UNDERGRADUATE
SCHOOL: CLEMSON UNIVERSITY

ELEAZAR MORA

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF HOUSTON

EDUARDO NEVAREZ

PROGRAM: UNDERGRADUATE
SCHOOL: NORTHERN NEW MEXICO COLLEGE

URIAH SANCHEZ

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF NEW MEXICO

GROUP: PM-DO
MENTOR: ROILYNN KNIGHT (LYNNE)
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: GROUP PRESENTATION
LA-UR-22-26580

IMPROVING LANL'S GROUND PENETRATING RADAR TECHNOLOGY

Whether it is starting a new building, or improving a new one, the Laboratory is always looking for the best technology to help with the job. Through this sustained work, there have been accidents that have occurred as a result of pre-construction site investigations. The goal of the summer 2022 ALDICP team was to determine and find better GPR technology in the market and from there, suggest new and improved technology to help prevent GPR-related accidents in the future. We aim to have a list of suggestions for the GPR team to implement which will, altogether, see to benefit the laboratory in the future to continue accomplishing its global mission to ensure the safety, security, and reliability of the U.S. nuclear deterrent.

ZACHARY KOEHN

PROGRAM: UNDERGRADUATE
SCHOOL: COLORADO SCHOOL OF MINES
GROUP: SIGMA 2
MENTOR: MICHAEL MCBRIDE
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27160

PYTHON-ATHON: AUTOMATION OF DATA PROCESSING

The electrochemistry and corrosion team in SIGMA-2 generates substantial materials science data, which needs to be processed in an efficient, user friendly, and reliable way. One dataset was a collection of corrosion images and standard corrosion data. Images were processed so that the code could find corroded surface areas and normalize the results. A second dataset collected real time electrolyte conditions. The code analyzed and graphed the data as it was recorded. Finally, the last set of data was thousands of Raman spectra. The code curve fits the data to four pseudo-voigt distributions and optimizes the parameters. Codes were written for these datasets that could take data, present it visually in a Graphical User Interface, (GUI), and analyze the data quickly with minimal user input.

PAUL LATHROP

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF CALIFORNIA, SAN DIEGO
GROUP: E-3
MENTOR: BETH BOARDMAN
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26956

QUANTUM COMPUTING APPROACHES TO RANDOM MOTION PLANNING

We recast traditional random motion planning algorithms into database-oracle structure to be solved via quantum amplitude amplification (QAA) for quadratic run-time speedup and future quantum implementation. For sparse environments, a database of possible full paths is created and searched using QAA. For dense 2D random square lattices, we formulate a quantum probabilistic road-map (QPRM) algorithm that creates and searches databases of possible parent-child connections to create a tree of reachable states. We numerically estimate the number of database solutions then provide algorithmic modifications to select the number of solutions. We compare the QPRM algorithm with a classical implementation and provide results in the largest connected component of a dense random lattice.

YU-HSUAN LEE

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF COLORADO BOULDER
GROUP: EES-17
MENTOR: ZHOU LEI
DISCIPLINE: ENGINEERING
SUBJECT AREA: GEOTECHNICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26698

MODELING PROJECTILE PENETRATION INTO SAND

The main aim of the project is to model projectile penetration into sand accounting for grain-scale fracture coupled to background gas, such as encountered in explosively loaded penetration into dry packed particle beds within the 800 MeV Proton Radiography facility at LANL. Different numerical methods, such as the discrete element method, the combined finite-discrete element method, and the computational fluid dynamics, are used. Approaches for upscaling of grain-resolved direct numerical simulation to Cauchy stress and large deformation measures are studied. This work will advance LANL's capabilities in understanding complex granular materials deformation events for advanced material model development within a proper nonlinear continuum mechanics constitutive modeling framework.

ZACHARIAH LEMKE

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF WISCONSIN-MADISON
GROUP: NEN-2
MENTOR: KELSEY AMUNDSON
DISCIPLINE: ENGINEERING
SUBJECT AREA: CRITICAL EXPERIMENTS
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27214

MODELING APPROACH TO CRITICAL IN THE UPCOMING CERBERUS EXPERIMENT

The Critical Experiment Reflected By copper to BettEr Understand Scattering [CERBERUS] is an integral experiment that will be executed at the end of FY23. The experiment is designed to study the intermediate energy range, in particular elastic and inelastic scattering of neutrons in copper. Approaching criticality safely is of utmost importance, and having a computer mode is a useful tool when determining changes that can safely be made to the experiment. Multiple simulations are needed to analyze the approach to critical, and manually creating MCNP input files is both tedious and error prone. To solve this problem, a python script was created to develop and run these input files.

LEI LIU

PROGRAM: GRADUATE
SCHOOL: THE UNIVERSITY OF TEXAS AT AUSTIN
GROUP: EES-16
MENTOR: BAILIAN CHEN
DISCIPLINE: ENGINEERING
SUBJECT AREA: PETROLEUM ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26934

REDUCED ORDER MODELS FOR GREENHOUSE GAS LEAKAGE USING MACHINE LEARNING METHODS

Geologic storage of carbon dioxide is a viable technique to combat climate change. Depleted hydrocarbons reservoirs are a promising candidate for storing carbon dioxide. However, these reservoirs contain residual contents of hydrocarbons that might become mobile during storage. Therefore, it is imperative to quantify the leakage risk of these hydrocarbons and carbon dioxide to shallow aquifers. Our project focuses on the leakage risk from wellbores which might provide potential leakage pathways. We propose developing Reduced-order models (ROMs) to enable fast and accurate predictions of leakage through wellbores. We examined the performance of various ROM development techniques, including multivariate adaptive regression splines (MARS), gradient boosting, and neural networks.

VIRGINIA LUCAS

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF FLORIDA
GROUP: NEN-1
MENTOR: ROBERT WEINMANN-SMITH
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27195

OPTIMIZATION OF A MICROREACTOR FRESH FUEL MEASUREMENT SYSTEM FOR SEALED CORES

The United States is looking to deploy microreactors in the near future as domestic sources of clean energy. Microreactors have unique features which make it difficult to verify the presence of the nuclear material within. Tracking this material is required for domestic and international safeguards. Because microreactors are still in the design process, developers have the opportunity to incorporate safeguards by design. This work examines material control and accounting techniques to quantify fresh microreactor fuel.

CHRISTINE MATHEW

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS A&M UNIVERSITY
GROUP: NEN-1
MENTOR: JACOB STINNETT
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27219

CALORIMETRY MEASUREMENTS USING A THERMAL CAMERA AND INFRARED THERMOMETER

The purpose of this measurement activity was to determine whether a thermal camera could be used to effectively measure the amount of plutonium in a facility's inventory. If proven effective, this method would be desirable as its speed and low cost would be useful for rapid inventory checks, albeit at the cost of a significantly larger measurement uncertainty. The use of a thermal camera for this application was tested by dividing 11 different radioactive sealed sources packaged in identical containers into two sets, and taking several images of the different sections.

SAMUEL MCBURNETT

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF TEXAS AT AUSTIN
GROUP: W-10
MENTOR: LAURA CARTELLI

DISCIPLINE: ENGINEERING
SUBJECT AREA: GENERATIVE DESIGN
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27271

MODIFYING A NON-DOMINATING SORTING GENETIC ALGORITHM FOR RADIATION SHIELDING

Radiation shield design using the NSGA-II genetic algorithm coupled to MCNP, a radiation transport code, takes a substantial amount of time to converge to a solution set. Convergence tests were developed to determine when the design algorithm had reached a converged solution. These tests were then used to evaluate the effectiveness of modifications to the genetic algorithm implemented with the goal of decreasing the convergence time.

SACHI MITCHELL

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF WISCONSIN MADISON

JULIAN MARTINEZ

PROGRAM: UNDERGRADUATE
SCHOOL: NEW MEXICO INST OF MINING

GROUP: ISR-1
MENTOR: ERNST ESCH
DISCIPLINE: COMPUTING AND INFORMATION TECHNOLOGY
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: GROUP PRESENTATION
LA-UR-22-27305

LOW-LEVEL WASTE RECEPTACLE DESIGN

Presently, LANL uses standard order industrial waste receptacles for the removal of low-level radioactive waste. To remove the contaminated waste from this original receptacle, workers must lift waste bags weighing 20-30 lbs above head level to clear the rim of the receptacle. This work process causes repetitive use injuries which are costly for the employer. For an alternative design, it is important to reduce the amounts of pinch points so that the personal protection equipment of the workers does not get caught and workers do not get pinched or cut. Throughout this project, multiple preliminary designs have been constructed in SolidWorks using input from management and mentors in order to create different features and implements that aim to solve this ergonomics issue.

MICHAEL MORRIS

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS TECH UNIVERSITY
GROUP: AOT-RFE
MENTOR: MARIA BARRUETA
DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27224

HVCM LLC RESONANT TOPOLOGY

LANSCE uses forty-four specialized linear vacuum tube amplifiers, known as klystrons, along the 805 MHz RF system to amplify the beam to its final output power. The power supplies for these amplifiers are pulsed DC voltage sources. A new method of supplying these RF amplifiers is theoretically explored in the interest of system simplification and possible higher output efficiency. This power delivery system acts as a DC-AC-DC converter utilizing resonance. Through controlling the switching frequency of the input DC voltage and the value of components in the resonant tank, the gain of the circuit can be controlled and calculated. This mathematical analysis of resonant converters can become the basis of designing a new generation of power supplies for the 805 MHz RF amplifier system.

TIMOTHY OCKRIN

PROGRAM: UNDERGRADUATE
SCHOOL: HOUGHTON UNIVERSITY
GROUP: NEN-1
MENTOR: KATRINA KOEHLER
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26936

IMPROVED ANALYSIS TOOLS FOR DECAY ENERGY SPECTROSCOPY

Nuclear safeguards uses various methods of verifying the isotopic composition of samples. Decay Energy Spectroscopy (DES) is a novel method that accomplishes this by measuring total decay energy using high energy resolution (1–5 keV @ 5 MeV) microcalorimeters. Decay Energy Spectroscopy Analyzer (DESA) is a Python-based software with a graphical user interface that analyzes Pu, U, or other actinide DES spectra and compares with declared isotopic ratios. In U DES spectra, the U-236 peak contains U-235 escape peak interference. DESA accounts for this using the probabilities of other isolated U-235 escape peaks. With recently developed capabilities, DESA will be a user-friendly and versatile tool to analyze DES data from the new International Atomic Energy Agency-commissioned DES spectrometer.

LUKE OUKROP

PROGRAM: UNDERGRADUATE
SCHOOL: PURDUE UNIVERSITY
GROUP: NEN-2
MENTOR: TRAVIS GROVE
DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27216

DEVELOPING A NEW CRITICALITY SAFETY HANDS-ON-DEMO UTILIZING ZPPR PLATES

LANL's criticality safety class already includes three different hands-on-demos. These demos utilize the BeRP ball, the neptunium sphere and class foils. It is desired that a new hands-on-demo be added to the program that utilizes Zero Power Physics Reactor (ZPPR) plates. This is for the purpose of familiarizing the students more with plutonium and to be able to demonstrate more MAGIC MERV parameters and how they affect criticality. MAGIC MERV stands for mass, absorption, geometry, interactions, concentration, moderation, enrichment, reflection and volume. These nine physical properties all affect the criticality of a system. It is the objective of the demonstration to show to the students how each one affects criticality. It is this work that will design a new demonstration.

JUSTIN PASCHKE

PROGRAM: UNDERGRADUATE
SCHOOL: UNION UNIVERSITY
GROUP: W-DES
MENTOR: DENVER SMITH
DISCIPLINE: ENGINEERING
SUBJECT AREA: SYSTEMS ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26325

MBSE WITHIN SYSTEMS ENGINEERING APPLICATIONS

Model-based systems engineering (MBSE) is the method used to create models of complex systems in support of requirements, design, analysis, verification, and validation from the beginning of the conceptual design phase to the development and later life cycle phases. The models created make for a more efficient way to explore, update, and communicate system aspects to stakeholders; this effectively reduces and/or eliminates the dependence of document-based information. Although models are not a perfect representation to the system, they provide feedback and knowledge earlier than traditional implementation alone, which in turn increases the quality and transparency, raises confidence, and diagnoses issues earlier through the entire lifecycle of the product.

REBECA ROCHA

PROGRAM: HIGH SCHOOL
SCHOOL: LOS ALAMOS HIGH SCHOOL
GROUP: E-6
MENTOR: CHRISTINA HANSON, ANTHONY WHITTEMORE
DISCIPLINE: ENGINEERING
SUBJECT AREA: NONDESTRUCTIVE TESTING AND EVALUATION
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26921

UNDERSTANDING THE DETECTION LIMITS OF SMALL DENSITY DIFFERENCES USING CT

Most people are familiar with common forms of nondestructive testing, such as x-ray and computed tomography (CT) scans. One key issue with these specific tests is that it's hard to tell the difference between small discrepancies in an object's density. To determine the limit for what is detectable variance in density, we're using a phantom with densities that vary by, at most, 5%. Using CAD software to model said phantom, I'm able to simulate x-rays under multiple conditions through a program called aRTist. Selecting the most optimal setup from these simulated data, measurements of the phantom will be taken using CT and digital radiography (DR). From here, we'll analyze these images to find density differences and compare the experimental results with the simulations.

DIVYANSHU SHARMA

PROGRAM: GRADUATE
SCHOOL: GEORGIA TECH UNIVERSITY
GROUP: XCP-3
MENTOR: JERAWAN ARMSTRONG

DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26246

DEVELOPING PYTHON CODES FOR PROCESSING MCNP ELEMENTAL EDIT OUTPUTS

An MCNP transport code has the capability of tracking particles on unstructured mesh (UM) geometry models and tallying quantities of interests on finite elements. The MCNP code writes these quantities of interests into a file known as an elemental edit output (EEOUT) file. MCNP 6.3 can create two EEOUT file formats: ASCII and HDF5. The results in EEOUT files are typically processed for further analysis and/or multiphysics calculations, such as MCNP/Abaqus coupling calculations. An HDF5 EEOUT file format is a new feature in MCNP 6.3, and this project focuses on developing Python codes for post-processing HDF5 EEOUT files. A Python code has been developed to convert an MCNP HDF5 edit output type 6 (i.e., energy deposition) into a heat flux file format for an Abaqus heat transfer calculation.

ANTHONY JAMES SHAW

PROGRAM: UNDERGRADUATE
SCHOOL: CALIFORNIA STATE UNIVERSITY AT SACRAMENTO

ANA CLECIA ALVES ALMEIDA

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF AKRON

GROUP: UI-OSI
MENTOR: JORDAN BRENNER
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: GROUP PRESENTATION
LA-UR-22-27257

FEASIBILITY OF CARBON-FREE AND NET-ZERO ENERGY HEATING AND COOLING IN MULABS

Heat pumps have been shown to be an effective source of both heating and cooling, especially when paired with a clean energy source such as solar. This study models the heating and cooling needs for the Multi-use Laboratory Buildings (MULABs), a heat pump system sized for the building's heating and cooling needs, the electrical demand required to run the system, and the solar panel array extent to generate the power needed to offset the heat pump electrical demand. By comparing its efficiency and carbon neutrality with natural gas furnaces operations, we proved that heat pumps are effective in providing heating and cooling in the different seasons at Los Alamos. These efforts will help guide future building projects and support the campus wide net-zero plan.

KASSIDY SHEDD

PROGRAM: UNDERGRADUATE
SCHOOL: NEW MEXICO STATE UNIVERSITY
GROUP: MPA-Q
MENTOR: NICHOLAS DALLMANN
DISCIPLINE: ENGINEERING
SUBJECT AREA: SIGNAL PROCESSING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27112

USING THE KALMAN FILTER IN NAVIGATION PREDICTION WITH VEHICLE MOTION CONSTRAINTS

The Kalman Filter (KF) predicts a state (condition of variables at a certain time) based on the previous state, measurements, and a model of the system dynamics. In this project, the KF is used in vehicle navigation and position tracking by combining measurements from a representative vehicle field test, including acceleration values that have been rotated into a global reference frame with gravity subtracted, and GPS position measurements with simulated noise added. Effects of noise on KF performance are quantified by varying the simulated position measurement noise and comparing the KF result against the original GPS position measurements. The KF uses vehicle constraints such as largest possible acceleration and turn radius per time stamp to further refine the solution.

RACHEL SIMMS

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS A&M UNIVERSITY
GROUP: ISR-4
MENTOR: SUSAN MENDEL

DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26955

DIGITAL PULSE PROCESSING FOR RADIATION DETECTORS

This project focuses on digital pulse processing (DPP) for an energetic charged particle telescope to be used on a 12U CubeSat. This instrument enables measurements of energetic charged particle populations and energy-dependent spectra through the radiation belts. This project looks to digitize earlier in the signal chain and at higher speeds, with much of the signal processing in the digital domain. Doing so enables detection at higher event rates, better discriminating from background radiation, than if the filtering was strictly done through analog.

DANIELLE SOUTH

PROGRAM: GRADUATE
SCHOOL: TEXAS A&M UNIVERSITY
GROUP: NEN-1
MENTOR: SARAH SARNOSKI

DISCIPLINE: ENGINEERING
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26562

DIGITAL TWIN OF A HLNCC IN A DYNAMIC ENVIRONMENT

In order to control background, nuclear material is often transported from a working area into a shielded measurement area. While effective, material movement represents a significant contamination and exposure risk to operators This work aims to remove that step from the process and enable the use of high precision instruments in a dynamic environment. A methodology is demonstrated which uses dispersed neutron detectors in a mock glovebox environment to quantify a dynamic background count rate and remove it from an HLNC measurement. The effectiveness of this methodology is quantified experimentally by measuring the mass of a Cf-252 source in an environment where several other sources are moving throughout the room during the measurement.

GRANT STEVENSON

PROGRAM: GRADUATE
SCHOOL: GEORGIA TECH UNIVERSITY
GROUP: MPA-11
MENTOR: JOHN GREENHALL

DISCIPLINE: ENGINEERING
SUBJECT AREA: ACOUSTICS
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27259

SENSITIVITY ANALYSIS FOR EPOXY SELECTION AND ACOUSTIC COLLIMATION OPTIMIZATION

Generating a low-frequency Collimated Acoustic Beam (CAB) is desirable for acoustic imaging. Low-frequency acoustic waves lead to increased imaging distance, while collimation increases the image resolution. Prior work has shown that constraining the radial motion of a piezoelectric disk leads to an enhanced CAB. However, applying symmetric constraint is challenging in practice. In this study, we investigated radially constraining the disk using a hollow cylinder affixed via epoxy adhesive. The focus of this experiment was to study how the epoxy material properties affected CAB performance. Utilizing a design of experiments and COMSOL simulation, sensitivity analysis was performed to establish the relationships between the epoxy material properties and the resulting degree of collimation.

LUKE STREBE

PROGRAM: GRADUATE
SCHOOL: NEW MEXICO TECH UNIVERSITY
GROUP: ISR-1
MENTOR: ERNST ESCH (SHORTY)
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27306

AUTOMATED INSPECTION STAND FOR NUCLEAR WASTE DRUMS

Nuclear waste storage and management is vital for Los Alamos National Laboratory (LANL). Nuclear waste is stored in 55-gallon steel drums that need to be frequently monitored by a worker physically inspecting the drums. The current process for inspecting drums is in conflict with the LANL ALARA (As Low As Reasonably Achievable) program for radiation worker safety. An Automated Inspection Stand (AIS) was proposed to remove the need for workers to physically handle the drums. The AIS is designed to have each drum loaded by forklift onto the stand where the drum can rotate and be viewed by multiple cameras and sensors. Implementation of the AIS will put the worker at a further distance from the waste during the inspection process keeping in line with the ALARA program.

KAI SUMMERALL

PROGRAM: GRADUATE
SCHOOL: TEXAS TECH UNIVERSITY
GROUP: MPA-11
MENTOR: TOMMY ROCKWARD
DISCIPLINE: ENGINEERING
SUBJECT AREA: ENVIRONMENTAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27359

IN-LINE HYDROGEN CONTAMINATION DETECTOR

Impurities in hydrogen gas, such as carbon monoxide (CO), can poison PEM fuel cells by absorbing onto active platinum sites and thus reducing its overall performance. It becomes paramount to detect these non-hydrogen constituents before they enter the anode feed-stream. We are working developing am in- line hydrogen contamination detector (HCD) capable of sensing low levels of CO. The HCD must detect impurities in a dry hydrogen gas stream without the presence of water and oxygen. The HCD is composed of a polybenzimidazole (PBI) membrane, and two gas diffusion electrodes loaded with platinum catalyst. The detector's current response and impedance is monitored as the CO concentration varied.

YULIIA TRUJILLO

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF NEW MEXICO
GROUP: C-CDE
MENTOR: VICTORIA HYPES-MAYFIELD
DISCIPLINE: ENGINEERING
SUBJECT AREA: FUSION TECHNOLOGY
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27096

PERFORMANCE TESTING OF AN AIRSQUARED ALL-METAL SCROLL PUMP FOR FUSION FUEL CYCLE

Fusion power is released when deuterium (D) and tritium (T) collide and fuse into a helium-4 atom plus a high-energy neutron. The reactor exhaust will be processed to recover the unreacted D and T. Vacuum pumps are essential components of the process. These pumps should remediate risk of contamination of oils and polymers. Industry standard Normetex pumps are all metal, oil-free, hermetically sealed scroll pumps designed for use in fusion environments. Normetex has gone out of business, and AirSquared has developed a similar vacuum pump. Extensive research on the new pump was performed for a direct comparison to the Normetex with various gases. The flowrate was calculated from the experimental data, and the ultimate vacuum capability was analyzed and directly compared to Normetex data.

GERRIT VANDER WIEL

PROGRAM: UNDERGRADUATE
SCHOOL: LETOURNEAU UNIVERSITY
GROUP: W-13
MENTOR: PAULA RUTHERFORD
DISCIPLINE: ENGINEERING
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26924

EVALUATION OF BRAKE-REUB STRUCTURAL RESPONSE DUE TO VARIABLE CONTACT MODELING

Bolted surfaces are essential for the structural design of many systems such as aircraft and spacecraft body panels. However, these bolted structures have nonlinear mechanical responses when dynamic loading is applied, making structural response modeling difficult. Contact surfaces during dynamic loading exhibit phenomena such as micro-slip, nonlinear friction interactions, and vibrational damping contributing to the nonlinear effect. Finite element analysis was used to describe a simple lap joint in a beam (the Brake-Reuß beam) to help discover methods that best describe the vibrational response at varying impulse amplitudes. Care was taken to incorporate subtle, yet important aspects of the physical experimental setup into the structure model such as accurate bolt loading and boundary co.

ADITYA WAGHMARE

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS TECH UNIVERSITY
GROUP: AOT-RFE
MENTOR: THOMAS HALL (WES)
DISCIPLINE: ENGINEERING
SUBJECT AREA: ELECTRICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27229

201.25MHZ WINDOW TEST STAND EXPERIMENTAL ANALYSIS

This paper focuses on the Los Alamos Neutron Science Center 201.25MHz window test stand used for testing window performance for changes in input power, pressure variations and other coaxial window attributes. Three experimental set-ups were analyzed to compare the effect of window coatings. Analysis was focused on acquiring real test data, modeling this data and developing a CST simulation model. Data was collected via a C++ program and graphed in MATLAB. The measured data were peak power levels, pressure, and window temperatures, and these allowed us to identify correlations in the various test cases which were correlated to adverse phenomenon occurring inside the window test stand such as multipactor and ion bombardment. Thermal effects were examined in depth, including CST simulations.

HEALTH AND SAFETY

GEORGE ABERNATHY

PROGRAM: POST MASTERS
SCHOOL: BLACK HILLS STATE UNIVERSITY
GROUP: B-10
MENTOR: ANAND KUMAR

DISCIPLINE: HEALTH AND SAFETY
SUBJECT AREA: APPLIED MICROBIOLOGY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27028

A RAPID PHAGE ISOLATION PLATFORM FOR TARGETING ANTIBIOTIC-RESISTANT PATHOGENS

The WHO predicts antibiotic resistance (AR) in bacteria will kill over 300 million people and cost $100 trillion globally by 2050. Thus, phage therapy has generated renewed interest to solve this crisis—however, the conventional phage isolation methods are low-throughput, inefficient, and tedious. Here, we are developing 'RapidPhage,' a novel high-throughput microfluidic platform to isolate phages against any strain of bacterial pathogen. We are currently developing and testing RapidPhage to demonstrate superiority over conventional methods for isolating phages against AR pathogens. The developed RapidPhage platform will revolutionize the phage isolation method as classical isolation method once did at the beginning of phage research a century ago.

IAN THOMAS PARKER

PROGRAM: UNDERGRADUATE
SCHOOL: RENSSELAER POLYTECHNIC INSTITUTE
GROUP: XCP-7
MENTOR: LUCAS HETRICK
DISCIPLINE: HEALTH AND SAFETY
SUBJECT AREA: HEALTH PHYSICS
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27307

QUANTIFICATION OF ICRP 145 HUMAN PHANTOMS FOR CHARACTERIZING EXTERNAL RADIATION

The International Commission on Radiological Protection (ICRP) periodically publishes and updates Dose Conversions Factors (DCFs), ICRP Publications 74 and 116, which can be used in combination with the Monte Carlo N-Particle (MCNP) radiation transport code. Recently, ICRP Publication 145, released “adult mesh-type reference computational phantoms”, which provide detailed unstructured mesh human phantoms to be incorporated into the MCNP calculations, allowing dose to be directly calculated rather than relying upon DCFs. This work aims to quantify the calculational differences of the standard techniques of DCF’s in combination with constructive solid geometry (CSG) vs the human phantoms. These calculated radiological quantities will validate and quantify accuracy and precision of phantoms.

MATERIALS SCIENCE

DANIELLE ALVERSON

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF FLORIDA
GROUP: W-13
MENTOR: AMBER WHELSKY
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: COMPUTATION SCIENCES AND MACHINE LEARNING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26739

ASSESSING SURROGATE MODEL PREDICTIONS THROUGH UNCERTAINTY QUANTIFICATION

The goal of the summer project is to develop a way to investigate uncertainty associated with surrogate model predictions of two kinds of datasets. A surrogate model is used in order to mitigate the large number of computational resources by minimizing the required parameters and finding the relationship between parameters that describe the most significant aspects of data behavior. In this project, Prophet, a tool developed within the Advanced Engineering Analysis Group (W-13), along with other open-source python modules were used to build and assess surrogate models of; 1) example data generated from two known sensors and 2) stress output within the Brazilian Disk Dataset of three Polymer Bonded Explosive materials.

SAMUEL BODEN

PROGRAM: UNDERGRADUATE
SCHOOL: MIAMI UNIVERSITY- OXFORD, OH
GROUP: MST-16
MENTOR: SARAH HERNANDEZ

DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: NUCLEAR MATERIALS SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27217

INVESTIGATING THE ROLE OF DEFECTS IN THE ALPHA-BETA PHASE TRANSFORMATION OF PU USING DFT

Before reaching its relatively low melting point of 913K, Pu undergoes six solid state phases: simple monoclinic alpha, body-centered monoclinic beta, face-centered orthorhombic gamma, face-centered cubic delta, body-centered tetragonal delta-prime, and body-centered cubic epsilon phases. Due to their low-symmetry, the monoclinic alpha and beta phases have not been studied extensively, however it has been previously hypothesized that defects in the alpha lattice may facilitate the transition to the beta phase due to the incommensurate number of atoms. In this work, we use DFT to calculate how defects may be influencing the alpha-beta transition, where results indicate that interstitials induce beta features structurally and electronically, such as volume expansion and bonding changes.

PETER BRAEGELMANN

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF OREGON
GROUP: MST-7
MENTOR: JOSEPH TORRES
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: ADDITIVE MANUFACTURING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-25594

DEVELOPING A ROADMAP TO MANUFACTURE FEEDSTOCKS FOR SELECTIVE LASER SINTERING

An important goal for the National Nuclear Security Administration is to improve the agility and responsiveness to field new stockpile designs. Manufacturing of polymeric components for nuclear weapons applications is often performed by outside vendors via injection molding and machining. Recent problems with this strategy include failures in visual and dimensional inspections. Additive Manufacturing supports this goal by providing the ability to rapidly produce small lots of prototype components early in the production process, enabling development work for component maturation and insertion. In order to realize this goal, we seek to optimize custom powder feedstocks for SLS. This work focuses on developing a roadmap to process non-commercial materials into printable feedstocks.

TAYLOR BUCKWAY

PROGRAM: POST MASTERS
SCHOOL: BRIGHAM YOUNG UNIVERSITY
GROUP: C-PCS
MENTOR: PAMELA BOWLAN
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: MATERIALS SCIENCE
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27073

ULTRAFAST XUV EXCITATION FOR ALTERING MACROSCOPIC MATERIAL PROPERTIES

The advancement of ultrafast laser technology has opened the doors to control macroscopic material properties, such as magnetism and ferroelectricity, on a femtosecond time-scale. Such research could lead to new technology for faster computing and data storage. We are developing an intense tabletop XUV femtosecond light source, to explore ultrafast control of material properties in a new way, through shallow core electrons in materials. The tabletop source will have full polarization tunability, giving access to the spin of the electrons. We will do pump-probe experiments where the XUV beam will be the pump and an infrared beam will probe the macroscopic material property changes on a fs-timescale working towards the goal of ultrafast control of magnetism or ferroelectricity in solids.

JOSE COLON RIVERA

PROGRAM: GRADUATE
SCHOOL: DUKE UNIVERSITY
GROUP: NSEC-IMS
MENTOR: FILIP RONNING
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: MATERIALS SCIENCE/NUCLEAR PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27197

DFT CALCULATIONS OF F-ELECTRON QUANTUM MATERIALS FOR APPLICATIONS IN DARK MATTER

Quantum Materials are materials whose understanding requires a quantum mechanical treatment. As such, these systems exhibit exotic properties such as superconductivity, spin liquids, etc. The SPLENDOR Experiment is aimed at developing quantum materials for light dark matter detectors. Here, we carry out density functional theory (DFT) calculations of the narrow band gap materials Ba3Cd2As4 and La3Cd2As6. From the DFT calculations, we develop a low energy effective model which enables us to compute the dielectric function. Due to a small band gap, these materials are sensitive to light dark matter. Using the theoretically calculated dielectric function, we can obtain the dark matter-electron scattering cross-section and explore the parameter space of several dark matter models.

MATTHEW DESMITH

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF OREGON
GROUP: MST-7
MENTOR: MICHAEL BLAIR
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: POLYMER SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27072

STRENGTHENING POLYETHYLENE THROUGH RADIATION-BASED CROSSLINKING

Polyethylene (PE) is among the most common polymers in the world. However, PE not always suited to long-term use in high-stress environments. It is prone to creep and wear over time, and the compounding effects of these phenomena can cause PE components to fail altogether. Vulnerability to creep and wear can be lessened by crosslinking PE, therefore increasing its strength and removing the ability to flow. Three different polyethylenes were crosslinked via gamma irradiation: Densetec (HDPE), Tivar 1000 (UHMWPE), and Polystone M (UHMWPE). These PEs were irradiated to doses of 0, 150, 200, 250, and 300 kGy, and the changes to their thermal, mechanical, and chemical properties were monitored.

CARL FAUVER

PROGRAM: GRADUATE
SCHOOL: TEXAS A&M UNIVERSITY
GROUP: T-3
MENTOR: DARBY LUSCHER
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: COMPUTATIONAL SOLID MECHANICS
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26231

CRYSTAL PLASTICITY DAMAGE MODELING IN FLAG

Single crystal plasticity is a well-established field that describes the elastic-viscoplastic behavior of individual single crystals. This theory is largely based on the concept of crystallographic slip. When external tensile loads are applied, the single crystals can develop and grow voids to relax the hydrostatic stress, leading to ductile failure of the crystals. My summer project aims to implement and improve a dislocation-based crystal plasticity damage model into a LANL Hydrocode FLAG. This model was originally developed by my summer mentors Nguyen, Luscher, and my Ph.D. advisor Wilkerson in JMPS 2017. In addition to adding this new capability to FLAG, I am improving the structure and end-user usability of the prototype production model DiscoFlux originally developed by Luscher.

ZHANGXI FENG

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF NEW HAMPSHIRE
GROUP: T-3
MENTOR: RICARDO LEBENSOHN
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: COMPUTATIONAL MECHANICS AND MATERIALS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26569

MODELING SURFACE ROUGHNESS IN COPPER UNDER CYCLIC THERMAL LOADING

During normal operations, accelerator cavities—made of a polycrystalline metal with extremely flat surfaces— experience pulsed heating due to radio-frequency loss. This ultra-high-cycle thermal loading results in the development of surface roughness that affects the surface currents and reduces the operando lifetime of these cavities. A large-strain thermo-elasto-viscoplastic Fast Fourier Transform (LS-TEVPFFT) formulation has been coupled with the solution for heat conduction, adding thermo-mechanical effects that enable microstructure-sensitive predictions of surface roughness in polycrystalline copper under high-cycle thermal loading.

KIERYA FREIBOTH

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS TECH UNIVERSITY
GROUP: MST-16
MENTOR: MEGHAN GIBBS, MATTHEW HAYNE
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: MECHANICAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27159

BOUNDARY HEAT TRANSFER EXPERIMENTS AND DENSITY CALCULATIONS PROGRAMMING

Computer modeling is only as good as the data put into it. To get reliable data, an induction furnace heated a graphite cylinder assembly. I wrote a LabVIEW Program that records the temperature as the heat transfers through the cylinders and used the results to support computer modeling efforts. Next, a laser profilometer was used to find a coating thickness. Finally, the setup can be used to find the effect of coating thickness on the heat transfer properties of the graphite assembly. Immersion density techniques are a great way to obtain the density of a material, but the calculations are hard to do by hand. A computer program makes this process much easier. With help from older programs with the same goal, I developed a LabVIEW program that can output the calculated sample density.

JONATHAN GARCIA

PROGRAM: UNDERGRADUATE
SCHOOL: FLORIDA INTERNATIONAL UNIVERSITY
GROUP: MPA-11
MENTOR: TOMMY ROCKWARD
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: ACOUSTICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27334

ACOUSTIC MANIPULATION OF PLATINUM CATALYST IN FUEL CELLS

During production of Proton Exchange Membrane Fuel Cells (PEMFCs), a Platinum catalyst (Pt-Cat) in a liquid solution is sprayed over a polymer-electrolyte membrane (PEM). The Pt-Cat acts with the PEM as an anode and cathode as it can avoid catalyst and PEM degradation. Pt-particles used are in a pressurized plastic tube which are not held in suspension, causing a non-uniform distribution of particles on the PEM. Here we use acoustics to manipulate Pt-particles to identify whether glass or plastic tubes should be used. Once identified, optimization in the manufacturing process of PEMFCs is possible. Through manipulation of acoustic fields and resonance frequencies, particles can be maneuvered to fit specific purposes, either for alignment, or dispersing them uniformly in a liquid.

JASON GIBSON

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF FLORIDA
GROUP: T-1
MENTOR: JAN JANSSEN

DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: MATERIAL INFORMATICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26057

AN INFORMATION THEORY BASED APPROACH FOR TRAINING MACHINE LEARNED POTENTIALS

The promise of obtaining accuracy on par with 1st-principle calculations at the computational cost of empirical potentials has made machine-learned interatomic potentials (MLP) attractive alternatives for studying materials. While many MLP have reported accuracy within several meV/atom of 1st-principle data, performance on novel configurations can incur errors that are orders of magnitude larger. This work leverages a dataset of more than 7M atomic environments in Tungsten optimized to maximize its informational entropy, ensuring broad coverage compared to hand-crafted datasets. First, we investigate the test errors' dependence on the training set's size. We then compare strategies to optimally sub-select training from this dataset to maximize the transferability/cost of the resulting MLP.

ADRIAN GONZALES

PROGRAM: GRADUATE
SCHOOL: THE UNIVERSITY OF TEXAS AT SAN ANTONIO
GROUP: MST-8
MENTOR: JOSHUA WHITE

DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: HIGH DENSITY NUCLEAR FUELS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26819

ASSESSMENT OF HIGH-DENSITY FUELS DURING HYDROGEN INTERACTION

High-density fuels (HDF) are nuclear fuels that contain a higher uranium density than traditional uranium dioxide. Research of HDF focusing on the oxidation of U3Si2, UN, UC, and UB2 in air, water, and steam environments concluded uranium forms UO2 and U3Si2 forms a hydride. However, minimal research has been done on the interaction between HDF and hydrogen. The Sieverts technique is implemented in the present study to detect hydrogen absorption by monitoring pressure drops during the hydrogen interaction with HDF. The results presented cover a temperature range from 100 to 500 °C in up to atmospheric pressures for 24-96 hour dwells. The presented data will be discussed in relation to LWR fuel performance interactions with hydrogen containing atmospheres.

MD MEHADI HASSAN

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF NEW MEXICO
GROUP: MST-8
MENTOR: EROFILI KARDOULAKI
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27001

ADVANCED MATERIALS FOR NUCLEAR SMALL MODULAR REACTORS

Small modular reactors can meet the power needs of remote communities or disaster zones in a reliable, flexible, and cost-effective manner. Molybdenum-based alloys are good cladding candidate materials due to their high melting point, high thermal conductivity, and high strength at elevated temperatures. However, contact with the graphite core can its immense carbon diffusivity promote the formation of Mo2C at high temperatures which can be harmful to the overall mechanical integrity of the material. High temperature ceramic coatings could act as great diffusion barriers that protect the Mo-based alloy from carburization. Long-term graphite diffusion tests on pristine and coated Mo-based alloys with AlN and TaC reveal the both materials could be used to prevent carburization at 1000 °C.

ERIN HEILMAN

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF TEXAS AT AUSTIN
GROUP: XCP-2
MENTOR: NATHANIEL MORGAN

DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: LAGRANGIAN HYDRODYNAMICS MODELING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27014

MODELING METALS USING LAGRANGIAN HYDRODYNAMICS CODE ON MULTIPLE ARCHITECTURES

Shock hydrodynamics is used to understand the behavior of materials when they interact with a shock wave. Using Fierro, a Lagrangian, parallel hydrodynamics code, we can model the deformation of materials at high strain rates on both CPUs and GPUs. By writing a hypo-elastic plastic material model and Mie-Gruneisen equation of state into Fierro, we are able to model the deformation of a range of metals at high strains and impacts, here using the Taylor Anvil experiment as a metric. Utilizing the Kokkos implementation in Fierro, we are then able to achieve ~8 times speed up in calculation time by running the code on GPUs.

MARCOS HERNANDEZ

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF NEW MEXICO
GROUP: C-CDE
MENTOR: JOSEPH DUMONT
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: MATERIALS ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26869

USE OF WASTE BIOPRODUCTS AS A CO2 SINK IN SUSTAINABLE STRUCTURAL COMPOSITES

By identifying useful waste streams, bio-manufacturing technologies such as sustainable composite materials can be developed to offset CO2 emissions. Waste biomass offers many material advantages such as biosequestration, biomineralization, and improved mechanical properties. By incorporated bio-waste into cementitious, pressed, and hydrogel materials we aim to develop bio-composites for applications in structural materials, 3D printing, and fuel pellets. Samples were prepared and characterized using a wide range of chemical, mechanical, and spectroscopic techniques. From this study, we evaluated the effects of waste biomass in sustainable composites for CO2 mitigation, reduced construction cost, and waste utilization potential.

WAKEIYO HETTINGA

PROGRAM: UNDERGRADUATE
SCHOOL: LOS ALAMOS HIGH SCHOOL
GROUP: MPA-11
MENTOR: CORTNEY KRELLER
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: MATERIAL ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27260

OPTIMIZING GASKETS FOR PASSIVE FUEL CELL STACK OPERATION

The fuel cell group in MPA-11 is developing PEM fuel cells for specific NNSA applications through the proper combination of materials designed to meet specific parameters. Designs must account for the management of biproduct- H2O, sealing of reactants, and efficient diffusion of H2 and O2 onto the three-phase interface. This work focuses on the Uno fuel cell. The NNSA requires that this fuel cell supply 25 mW of power continuously for 2-3 years, under passive operation at -55 to 80˚C. As a result of the temperature variance and time frame of operation, the gasket (seal) used is crucial to the design of the Uno stack. Using water wicking analysis, environmental chamber thermal cycling, and performance test data, the sealing and passive water removal of the Uno stack will be determined.

LANDON JOHNSON

PROGRAM: GRADUATE
SCHOOL: NORTH DAKOTA STATE UNIVERSITY
GROUP: T-1
MENTOR: GALEN CRAVEN

DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: THEORETICAL CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26859

DATA-DRIVEN MODELS FOR DIFFUSIVITY IN NUCLEAR FUELS

The generation of atomistic structural defects can significantly alter the performance characteristics of a nuclear fuel. This alteration of functionality often opens questions related to the fuel's readiness at various stages of the energy pipeline. Understanding and predicting how defects form and move through the atomistic lattice of the fuel is therefore of significant importance in both the design of new nuclear fuels and the assessment of current fuel stockpiles. In this talk, I will show my work applying machine learning methods to determine the diffusivity of various atomic species in uranium oxide and uranium nitride. I will show how machine learning can increase the accuracy of diffusivity prediction in nuclear fuels in comparison to the current state-of-the-art models.

SANGWON LEE

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF MICHIGAN
GROUP: MST-8
MENTOR: REEJU POKHAREL
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: MATERIALS SCIENCE ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27378

HYDROGEN EFFECTS ON ADDITIVELY MANUFACTURED STEEL USING HIGH-ENERGY X-RAYS

Hydrogen is deleterious in steel as it degrades mechanical properties causing loss of ductility and strength. In this work, we have used X-ray tomography and powder diffraction to characterize microstructural features of hydrided and non-hydrided additively manufactured and forged steel samples. The porosity evolution before and after tensile loading is characterized using X-ray tomograph and elastic lattice strains and lattice parameters evolutions were measured using powder diffraction. Also, notched samples were used to investigate crack initiation, crack propagation, and phase fraction evolution with cyclic loading, across the notch region. Experimental observations provide new insight into the effects of hydride on mechanical properties of steel with different microstructure features.

SOFIA PINZON

PROGRAM: GRADUATE
SCHOOL: FLORIDA INTERNATIONAL UNIVERSITY
GROUP: MPA-11
MENTOR: CORTNEY KRELLER
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: THIN FILMS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27111

PROCESSING EFFECTS ON THE MORPHOLOGIES OF CO-DEPOSITED SESQUIOXIDE THIN FILMS

Lanthanide sesquioxides are a material of interest for electronic, optical, and chemical applications. In the future, they may serve as a candidate material for an alternative gate dielectric due to their unique properties. Controlling and predicting the morphology of these complex oxides in thin film form is vital to their application in the above-mentioned applications. In the present study, single and co-deposited Er2O3, Lu2O3, and Sm2O3 thin films were grown on YSZ (8%) substrates by radio frequency (RF) magnetron sputtering at room temperature and 500°C. Both substrate temperature and target composition contributed to changes in crystallinity and grain structure which can enhance the chemical and physical properties of the films for their applications.

EMILY PROEHL

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF TENNESSEE- KNOXVILLE
GROUP: MPA-CINT
MENTOR: CALVIN LEAR

DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: MATERIALS SCIENCE AND ENGINEERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27348

IN-SITU TEMPERING DURING AM TO TAILOR GR91 STEEL REACTOR COMPONENTS

Reducing costs of in-core components is imperative for the feasibility of next generation nuclear reactors. High service temperatures also require creep resistant materials, such as ferritic/martensitic Grade 91 (Gr91) steel (9Cr-1Mo-V-Nb). Laser additive manufacturing (LAM) of Gr91 steel with in-situ tempering is a promising alternative to produce the desired tempered martensite microstructure and net shape parts without time- and energy-intensive heat treatment or machining needed for conventional production. This work compares Gr91 steel microstructural features from various LAM builds using scanning electron microscopy (SEM) to determine: a) the connection between microstructure and thermal cycles during LAM, and 2) how to tailor build parameters for LAM Gr91 steel reactor components.

GERONIMO ROBLES

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF TEXAS AT SAN ANTONIO
GROUP: MPA-8
MENTOR: JOSHUA WHITE
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: NUCLEAR FUEL MATERIALS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26984

THERMOMECHANICAL PERFORMANCE OF AL ANDAL2O3 ALLOYED FUELCOMPOSITE U3SI2+50WT%UB2

Progress in advanced nuclear fuel development of high density fuel (HDF) composites like U3Si2/UB2 as a drop-in replacement for conventional UO2 has been pursued for their superior uranium density and thermal conductivity. However, mitigating the potential for the energetic pulverization of U3Si2 during exposure to high temperatures and oxidants during potential off- normal conditions remains. This work details efforts to further improve the performance of U3Si2 + 50wt% UB2 by Al alloying for oxidation resistance and Al2O3 oxide dispersion strengthening to increase fracture toughness. Arc melted ingots and pellets, in as fabricated and annealed conditions, are subjected to high temperature steam oxidation and nanoindentation. Microstructure evolution is characterized via SEM/EDS and XRD.

JESSICA STANFEL

PROGRAM: UNDERGRADUATE
SCHOOL: COLORADO SCHOOL OF MINES
GROUP: PT-4
MENTOR: MEAGAN WHEELER

DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: MATERIALS SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26831

MICROSTRUCTURAL ANALYSIS OF BI-SN EUTECTIC

Analysis of a Bi-Sn eutectic will be completed through the usage of a graphite wedge mold. The wedge mold will allow for three distinct regions to form. These three regions will be analyzed for key microstructural features. In addition to this analysis, impact of coating on the microstructure will also be considered for the study. Two casts will be completed with one cast being completed without mold coating and the second cast will have a Yttria coating on the graphite mold.

XAVIER TORRES

PROGRAM: POST BACHELORS
GROUP: C-CDE
MENTOR: SHELBIE LEGETT
DISCIPLINE: MATERIALS SCIENCE
SUBJECT AREA: POLYMER ADDITIVE MANUFACTURING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26801

PRINTABILITY AND TESTING OF RADIATION SHIELDING POLYMERS

Radiation shielding has historically been accomplished using materials such as lead (Pb), which is problematic due to its weight and health/environmental issues. The work I am doing is attempting to address these issues through the creation of radiation-shielding polymers via Direct-Ink-Writing (DIW). The DIW resins in which we work with include W, WO_3, and Gd_2O_3 fillers, which act as radiation shields without the detrimental effects associated with Pb. During the printing stages, the resins are made in various wt% formulations to compare properties at the differing percentages. Determination of the printability and overall mechanical performance of these resins are achieved by printing and characterizing circular pads with a face-centered tetragonal or square centered lattice structure.

MATHEMATICS

LUCAS BLAKESLEE

PROGRAM: HIGH SCHOOL
SCHOOL: SANTA FE HIGH SCHOOL
GROUP: CCS-6
MENTOR: JUSTIN STRAIT, JEFFREY HYMAN
DISCIPLINE: MATHEMATICS
SUBJECT AREA: GRAPH THEORY
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26948

KERNEL EVALUATIONS OF SPECTRAL GRAPH SPARSIfiCATION ON DISCRETE FRACTURE NETWORKS

Sparsification of large networks is often necessary to make them computationally tractable. One area where this is relevant is the study of subsurface discrete fracture networks for fractured solids, including particle flow and transport. We apply an effective-resistance-based spectral algorithm to sparsify graph representations of these networks. Varying degrees of sparsification are applied to test the extent to which graphs can be reduced while maintaining properties of interest. Comparisons are performed using graph kernels, namely the multiscale Laplacian graph kernel and the "GraphHopper" kernel, to illustrate the amount by which graphs can be sparsified while still maintaining a high degree of similarity to their parent graphs, as well as preserving flow and transport calculations.

AMBER DAY

PROGRAM: GRADUATE
SCHOOL: THE UNIVERSITY OF TEXAS AT AUSTIN
GROUP: CCS-6
MENTOR: NATALIE KLEIN
DISCIPLINE: MATHEMATICS
SUBJECT AREA: STATISTICS
TYPE: INDIVIDUAL

LA-UR-22-25874

DETECTING SYNTHETIC OPIOIDS WITH NQR SPECTROSCOPY AND SIGNAL DENOISING

Dangerous synthetic opioids (e.g. fentanyl) are known to be synthesized abroad and shipped into the United States illegally via international mail. The aim of this research is to help reduce the flow of these drugs into the United States by developing a technology capable of detecting the presence of fentanyl in unopened packages using Nuclear Quadrupole Resonance (NQR) spectroscopy. NQR technology uses radio-frequency signals to detect if certain chemicals are present in a package. However, the raw NQR measurements are complex-valued time series corrupted by noise. We develop statistical and machine learning approaches, including complex-valued neural networks, and apply them to signal denoising allowing us to better determine whether chemicals of interest are present in a package.

JIHYEON KWON

PROGRAM: POST MASTERS
GROUP: CCS-6
MENTOR: KIMBERLY KAUFELD
DISCIPLINE: MATHEMATICS
SUBJECT AREA: STATISTICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27277

A TIME-VARYING OCCUPANCY MODEL FOR HISTOPLASMA IN THE U.S. USING EBIRD DATA

In the United States, the geographic distribution of environmental fungi that can cause fungal diseases is poorly understood. Histoplasmosis is a disease caused by the inhalation of the fungus, Histoplasma capsulatum, and can range in severity from asymptomatic to severe. However, the geographical distribution of the disease is not well known due to the limitations in public health surveillance. In this project, a Bayesian occupancy model utilizing space and time-varying variables is constructed using the citizen science data, eBird, while tackling the spatial bias and missingness issues in the eBird data. The model also introduces a seasonal occupancy component to provide awareness when there is a higher probability of the presence of Histoplasma capsulatum.

KATHERINE LI

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF MICHIGAN
GROUP: A-1
MENTOR: SARA DEL VALLE
DISCIPLINE: MATHEMATICS
SUBJECT AREA: DATA SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26421

ACCOUNTING FOR SPATIAL AUTOCORRELATION IN DISEASE MODELING FEATURE SELECTION

Predictive models of infectious disease burden are imperative for understanding the dynamics and developing mitigation efforts. However, the abundance of possible covariates presents a feature selection challenge. Further, heterogeneous data streams collected from a large region likely exhibit spatial autocorrelation, which may incur prediction bias and incorrect statistical inference if unaccounted for in model fitting. We propose an extension of feature selection via regularized regression that incorporates eigenvector spatial filtering to capture the data's spatial structure. We apply our method to severe acute respiratory illness (SARI) time series outbreak data across Brazil to identify predictors of SARI activity that can inform modeling and forecasting efforts.

OWEN PANNUCCI

PROGRAM: UNDERGRADUATE
SCHOOL: THE UNIVERSITY OF NEW MEXICO
GROUP: NEN-1
MENTOR: ROLLIN LAKIS
DISCIPLINE: MATHEMATICS
SUBJECT AREA: APPLIED MATHEMATICS/COMPUTER SCIENCE
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26564

ALGORITHM FOR MASS PREDICTION OF A NUCLEAR SOURCE IN A DYNAMIC ENVIRONMENT

To control background, nuclear material is transported from a working area into a shielded measurement area. While effective, material movement represents a large contamination and exposure risk. This work aims to remove that step from the process and enable the use of high precision instruments in a dynamic environment. A crucial procedure in this methodology is to accurately estimate the mass of the nuclear material source based on neutron rate output post background subtraction. The high-level neutron-coincidence-counter will be used to measure the nuclear material item and has a specific detector efficiency which will be considered when taking measurements. A non-linearity of source strength to mass ratio will also need to be taken into account to create a model for our HLNCC.

JENNIFER VACCARO

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF ILLINOIS CHICAGO
GROUP: XCP-4
MENTOR: ANGELA HERRING
DISCIPLINE: MATHEMATICS
SUBJECT AREA: COMPUTATIONAL PHYSICS
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26237

APPLYING AN ORIENTED DIVERGENCE THEOREM TO SWEPT FACE REMAP

We present a novel oriented divergence theorem and apply the results to swept face remap in ALE hydrodynamics. In our setting, we compute the material flux along swept regions between corresponding faces in the source and target mesh. Since the swept region may add material, subtract material, or intersect itself, we cannot apply divergence theorem without accounting for orientation. In this work, we encode the swept region orientation and geometry with a map from the unit cube, and then apply an oriented analog of divergence theorem to compute the material flux. To address our setting, we present efficient implementation strategies for swept face remap. We also provide numerical evidence supporting our results and discuss extensions to more general mesh topologies.

OTHER (NON-TECHNICAL)

ISHA DOGRA

PROGRAM: GRADUATE
SCHOOL: GEORGIA INSTITUTE OF TECHNOLOGY

TALA

PROGRAM: POST MASTERS
SCHOOL: UNIVERSITY OF ARIZONA

THOMAS JISTEL

PROGRAM: GRADUATE
SCHOOL: TEXAS A&M UNIVERSITY

GROUP: UI-OSI
MENTOR: GENNA WALDVOGEL
DISCIPLINE: OTHER (NON-TECHNICAL)
SUBJECT AREA: WATER MANAGEMENT AND PLANNING
TYPE: GROUP PRESENTATION
LA-UR-22-26088

WATER: WATER ASSESSMENT & TECHNICAL EFFICIENCY REPORT

With climate change and increasing water resource demands, it is vital to reduce consumption and use alternative sources to ensure water availability and critical infrastructure safety. The Water Management Team is creating a water balance to ascertain site-wide water flows for LANL and analyze current and forecasted water use across the campus. We will then recommend five-year water efficiency projects backed by feasibility studies to reduce consumption under various performance and financial constraints, while finding creative ways to meet current demands, and plan for future demands. These projects coincide with the latest Executive Orders, thus helping LANL meet water conservation goals for this decade by creating an implementation plan with institutional goals and policies.

SOFIA HORN

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF NEW MEXICO
GROUP: A-1
MENTOR: LORI DAUELSBERG

DISCIPLINE: OTHER (NON-TECHNICAL)
SUBJECT AREA: DATA SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27034

ANALYZING TRAVEL PATTERNS AND ACTIVITIES IN THE US

The National Household Travel Survey (NHTS) collects information about people's travel schedules and other aspects of daily life. My goal this summer was to analyze activities, travel patterns, and demographics to better understand the survey. I interpreted and visualized survey data in Python to learn about common trends in transportation based on how people respond. TRANSIMS—a LANL-developed agent-based model simulating transportation systems—will use this data to create activities and travel patterns for the United States. I found that activity patterns differ according to demographics, but their activities and where they go have little correlation to location and other unique aspects.

EDWARD KENDALL

PROGRAM: GRADUATE
SCHOOL: MOSCOW STATE INSTITUTE OF INTERNATIONAL RELATIONS/MIDDLEBURY INSTITUTE OF INTERNATIONAL STUDIES
GROUP: A-2
MENTOR: SHANNON JOHNSON
DISCIPLINE: OTHER (NON-TECHNICAL)
SUBJECT AREA: NONPROLIFERATION BIOECONOMY ISSUES
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26754

BIOREACTORS: MAKING BEER AND BUGS

Bioreactors are a means of growing microorganisms in large quantity and compose a category of inherently "dual-use" technologies: holding both immense potential for benefit and harm to society. Due to this duality, nonproliferation professionals must bridge technological understanding and policy acumen to see how bioreactors are integrated into both, many peaceful applications ubiquitous in the global bioeconomy such as in developing and manufacturing life-saving pharmaceuticals, as well as, potentially harmful and/or illicit uses, such as producing biowarfare agents.

SYDNEY MANGINELL

PROGRAM: UNDERGRADUATE
SCHOOL: NEW COLLEGE OF THE HUMANITIES
MENTOR: LAURA MCGUINESS

CATARINA TCHAKERIAN

PROGRAM: GRADUATE
SCHOOL: NORTHEASTERN UNIVERSITY
MENTOR: ALAN CARR

WILLIAM MASON

PROGRAM: UNDERGRADUATE
SCHOOL: ST. JOHN'S COLLEGE
MENTOR: NICHOLAS LEWIS

GROUP: WRS-NSRCMS
DISCIPLINE: OTHER (NON-TECHNICAL)
SUBJECT AREA: HISTORY AND PRESERVATION
TYPE: GROUP PRESENTATION
LA-UR-22-26830

THE FUTURE OF LANL'S NITRATE FILM COLLECTIONS

Cellulose nitrate was the first film base used for motion pictures and still images. Over 180 million feet of nitrate motion picture film reside in film archives globally, but nitrate film poses many challenges for archivists. It decomposes at unpredictable speeds and emits toxic gasses, endangering its historic value and the safety of surrounding holdings and archivists. Research following nitrate film's discontinuation in 1951 has discovered several ways in which nitrate film can be stored, preserved, and made available for viewing. By exploring the history of nitrate film, we hope to demonstrate the significance of the lab's nitrate holdings and preservation efforts, and to illustrate how the NSRC's work to make these collections accessible benefits LANL employees and researchers.

GABRIELLA SMITH

PROGRAM: POST BACHELORS
GROUP: CAS
MENTOR: PAUL ZIOMEK
DISCIPLINE: OTHER (NON-TECHNICAL)
SUBJECT AREA: VISUAL DESIGN AND MOTION GRAPHICS
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-27270

DESIGN IN MOTION: BRINGING LANL TO LIFE WITH ANIMATION

The overarching goal of my work is to use animation and design elements to create engaging and informative content to explain, and educate, or promote a wide range of work being done all around the lab. The scope of my work can range from simplified explainer animations to detailed scientific renderings. Regardless of the level of technicality, All content is based around a unique narrative that tells the story of the work being done and its importance, all while embodying the voice and spirit of the lab as a whole.

JUAN SURIEL

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF SOUTH CAROLINA
GROUP: EPC-WMP
MENTOR: DEBORAH WILLIAMS
DISCIPLINE: OTHER (NON-TECHNICAL)
SUBJECT AREA: WASTE MANAGEMENT TRACKING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27255

PRESENTING THE WASTE COMPLIANCE AND TRACKING SYSTEM (WCATS) DATABASE AT THE LANL

The purpose of this poster presentation is to provide information on the current and new formats of LANL's waste management database, WCATS legacy and WCATS3 respectively. The presentation will also be going into detail on some of the elements of the record keeping and tracking of waste generated at the laboratory from its creation to its disposition, how that process takes place and how our team ensures that waste generators adhere to the lab's regulations. To conclude, user feedback of the database that was obtained from daily WCATS users, primarily Waste Management Coordinators will also be mentioned and how this vital feedback will be utilized to benefit the developing WCATS 3 platform and optimize the management of waste here at LANL from cradle to grave.

PHYSICS

KEVIN ALLEN

PROGRAM: GRADUATE
SCHOOL: RICE UNIVERSITY
GROUP: T-4
MENTOR: JIANXIN ZHU
DISCIPLINE: PHYSICS
SUBJECT AREA: CONDENSED MATTER
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26214

FIRST PRINCIPLE STUDY OF ELECTRONIC STRUCTURE AND MAGNETISM IN COPT FORCATALYSIS

In this work, we focus on the CoPt material systems due to their enhanced magneto-crystalline anisotropy and high catalytic behavior. Particularly by performing first-principles electronic structure calculations, we will explore the Co moment response and the change of the coupling between molecules (e.g. O2) and the catalyst compounds to the effect of different surface orientations. This will be followed by simulating the inclusion of oxygen at different absorption angles on the surface to understand the catalyst interaction with the molecules. This study will allow a better understanding of the chemical reaction pathway and magneto-regulation activities in CoPt.

THAI HANG CHUNG

PROGRAM: GRADUATE
SCHOOL: BOWLING GREEN STATE UNIVERSITY

RILEY FERGUSON

PROGRAM: GRADUATE
SCHOOL: BOWLING GREEN STATE UNIVERSITY

SAMIKSHYA PRASAI

PROGRAM: POST MASTERS
SCHOOL: BOWLING GREEN STATE UNIVERSITY

GROUP: MST-8
MENTOR: YONGQIANG WANG
DISCIPLINE: PHYSICS
SUBJECT AREA: NUCLEAR MATERIALS
TYPE: GROUP PRESENTATION
LA-UR-22-27353

DEVELOPMENT OF AN IN-SITU POSITRON ANNIHILATION SPECTROSCOPY

Positron Annihilation Spectroscopy (PAS) is a set of techniques that non-destructively probe atomic scale vacancies and voids. As part of FUTURE EFRC, PAS will play a very important role in studying the evolution of defects in materials under irradiation, stress, and corrosion. We present the development of an in-situ pulsed variable energy positron beamline at LANL's IBML. The positron beam is coupled to a dual-beam irradiation chamber that uses a heavy ion beam from the 3 MV tandem accelerator for displacement damage production and also uses a He/H ion beam from the 200 kV ion implanter for emulating gas production by fast neutrons in advanced nuclear systems. The preliminary results from 3 MeV Fe ion beam damaged single crystalline Fe samples with 15 keV positron beam are reported.

FILIPPO DELZANO

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF CALIFORNIA- SANTA BARBARA
GROUP: T-2
MENTOR: EMANUELE MEREGHETTI
DISCIPLINE: PHYSICS
SUBJECT AREA: PARTICLE PHYSICS
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26932

CHARGED LEPTON FLAVOR VIOLATION IN HIGH ENERGY ELECTRON-PROTON SCATTERING

Since the discovery of the muon (μ) in 1936, the search for Charged Lepton Flavor Violation (CLFV) has been an intriguing avenue for the discovery of new physics. Its detection would not only improve knowledge of the Standard Model, but provide insight on other fundamental questions such as the origin of the neutrino's mass. Here, I present a preliminary analysis of the potential sensitivity of the Electron-Ion Collider (EIC) to CLFV in the $ep \rightarrow \mu X$ channel. I perform Monte Carlo simulations and detector-based analysis of high-energy signal and background Standard Model events and suggest certain cuts to enhance the estimated signal efficiencies. I conclude with a comparison to low-energy physics in order to identify competitive channels through which the EIC may hope to detect CLFV.

MATTHEW DEUTSCH

PROGRAM: GRADUATE
SCHOOL: KENT STATE UNIVERSITY
GROUP: XCP-2
MENTOR: EUNMO KOO
DISCIPLINE: PHYSICS
SUBJECT AREA: LAGRANGIAN PARTICLE PHYSICS, GPU PROGRAMMING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27084

SPEEDING UP LAGRANGIAN PARTICLE MODULES IN HIGRAD USING OPENACC

HIGRAD is a computational fluid dynamics model which can be used to simulate the cloud physics of pyrocumulonimbus (PyroCB) and localized weather systems caused by large-scale wildfires. HIGRAD uses an Eulerian approach for the atmospheric flow and a Lagrangian particle module for evolution/interactions of aerosols and cloud particulates, which are important for the study of PyroCBs and their impact on climate. The Lagrangian approach is better for complex particle physics models (e.g. collisions) but computationally expensive. We aim to improve the performance of the Lagrangian particle module using OpenACC, a compiler-directive based API for CPU and GPU parallelism. OpenACC requires minimal modification of the original program, leading to less intensive rewrites to introduce parallelism.

ETHAN FISK

PROGRAM: UNDERGRADUATE
SCHOOL: RENSSELAER POLYTECHNIC INSTITUTE
GROUP: XTD-IDA
MENTOR: JARRETT JOHNSON
DISCIPLINE: PHYSICS
SUBJECT AREA: ASTROPHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26927

AN IMPLEMENTATION OF FLUX ACCRETION FOR BLACK HOLES IN THE ENZO COSMOLOGY CODE

Using the Enzo cosmology code, we seeded a black hole at z=20 with an initial mass of 10^5 solar masses in a dark matter halo of mass ~4*10^7 solar masses. We tracked black hole accretion under different prescriptions as the halo grew to a mass of ~10^9 Solar masses by z=10. Accretion based on alpha disk formalism (DeBuhr et al. 2010), Bondi-Hoyle accretion (Bondi et al. 1952), and Bondi-Hoyle accretion modified to take vorticity into account (Krumholz et al. 2004), were modeled, with and without the Eddington limit. We modeled radiative transfer feedback from the blackhole with UV and X-Ray radiation. Accretion was also modeled using a new prescription based on the mass flux across the borders of the cell in which the black hole resides. We present the results from these prescriptions.

EMILY HOLMES

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF CALIFORNIA, BERKELEY
GROUP: XCP-2
MENTOR: DAVID CULP

DISCIPLINE: PHYSICS
SUBJECT AREA: COMPUTATIONAL PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27294

HIGH EXPLOSIVE SHOT MODELING AND FRAGMENTATION ANALYSIS IN PAGOSA

Experiments performed in 2020 by M-3 quantified the performance of U6Nb across hubcap and cylinder geometries. We simulate these experiments in the PAGOSA hydrocode to validate the FLIP+MPM Lagrangian capability and to improve fragmentation predictions. Several diagnostics are used to compare experimental and simulated results including Photon Doppler Velocimetry (PDV) and radiography. While PDV comparisons are readily quantitative, a metric derived from the radiography called the open area fraction needs to be post processed to provide a quantitative comparison of fragmentation. This derived quantity can be calculated using the Bayes Inference Engine and LaPlacian-of-Gaussian method. By varying simulated parameters, we provide validation of PAGOSA with FLIP+MPM using these diagnostics.

MATTHEW HOLMES

PROGRAM: POST MASTERS
SCHOOL: UNIVERSITY OF CALIFORNIA, SANTA CRUZ
GROUP: XCP-8
MENTOR: WENDY CALDWELL
DISCIPLINE: PHYSICS
SUBJECT AREA: IMPACT CATERING
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26452

MODELING MICROMETEORITE BOMBARDMENT INTO METAL TARGETS USING THE FLAG HYDROCODE

We are using the FLAG hydrocode to model micrometeorite bombardment into metal targets. We are interested in micrometeorites with diameter on the order of 100 microns and impacts of about 5 kilometers per second. Target materials of interest include aluminum, copper, tin, glass, and Pyrex (borosilicate glass), while carbon, ceramics, concrete, and silicates are being considered for the projectile's composition. Ultimately we are interested in repeated as well as nearly simultaneous impacts into a single target. To this end, we will study impacts into existing microcraters, as well as initialize simulations with multiple impactors to strike a single target. Currently, we have results only for fluid Al-Al impacts.

BRENDAN KING

PROGRAM: GRADUATE
SCHOOL: UNIVERSITY OF MINNESOTA
GROUP: T-2
MENTOR: INGO TEWS
DISCIPLINE: PHYSICS
SUBJECT AREA: NUCLEAR THEORY AND ASTROPHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26896

SYSTEMATIC BIASES WHEN INFERRING THE NUCLEAR EQUATION OF STATE FROM ASTROPHYSICS

The goal of this project is to constrain the true nuclear equation of state (EoS) via Bayesian inference with information encoded in the observed multi-messenger signal from merging NSs. We generate sample EoSs avoiding as many approximations as possible by drawing sample curves in the EoS space directly. The samples are constrained at low densities by state-of-the-art theoretical calculations performed at LANL and extended to higher densities in several ways. Data from observations encode neutron star parameters in the form of the mass, radius, and tidal deformability which we relate to the true EoS through the Tolman-Oppenheimer-Volkoff equations. By probing the true EoS with observations, we constrain the space of possible EoSs using PyCBC and pick the samples that agree best with data.

ANTHONY LESTONE

PROGRAM: UNDERGRADUATE
SCHOOL: TEXAS A&M UNIVERSITY
GROUP: P-3
MENTOR: JOHN MATTHEW DURHAM
DISCIPLINE: PHYSICS
SUBJECT AREA: PARTICLE PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26376

CONSTRAINING THE B QUARK HADRONIZATION MECHANISM

This project focuses on the study of B meson production in 13 TeV proton-proton collisions at the Large Hadron Collider measured with the LHCb experiment. The measured production rate of differently flavored B mesons was compared to monte carlo simulations. Simulation software contains only well-studied hadronization methods (fragmentation), so discrepancies between simulations and experimental data could imply the observation of novel hadronization methods (quark coalescence).

MENGKE LI

PROGRAM: GRADUATE
GROUP: T-CNLS
MENTOR: MATTHEW MUMPOWER
DISCIPLINE: PHYSICS
SUBJECT AREA: NUCLEAR ASTROPHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27126

NUCLEAR MASS WITH MACHINE LEARNING AND APPLICATION TO ASTROPHYSICAL R-PROCESS

The relation between the r-process abundance and the mass model has been investigated in previous study, and it was found that different mass models have strong influences on the calculated abundance pattern. However, the uncertainty of masses on the abundance pattern has not been investigated. We use a sophisticated Machine Learning based mass model utilizing the probabilistic Mixture Density Network to get the masses with quantified uncertainties of each mass. We predict the r-process abundance uncertainties that arise from the propagation of nuclear mass uncertainties. We also provide a more realistic abundance uncertainty distribution of heavy nuclei as compared with current approaches. The results of our work will inform the priority of the next generation of mass measurements.

ANH (KEN) LUU

PROGRAM: GRADUATE
SCHOOL: SAN FRANCISCO STATE UNIVERSITY
GROUP: CCS-2
MENTOR: NICOLE LLOYD-RONNING
DISCIPLINE: PHYSICS
SUBJECT AREA: ASTROPHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26553

GAMMA-RAY BURSTS AND BINARY PROGENITORS

Gamma-ray bursts (GRBs) are the most luminous objects in the universe. The duration of the prompt gamma-ray emission reflects how long a relativistic jet lasts in the black hole (BH) accretion disk system that powers GRBs. This quantity provides information about the amount of mass in the disk, the angular momentum in the BH disk system, and it is linked to properties of the progenitor system. We examine the possibility that longer lasting GRBs result from a massive star that collapses in an interacting binary system (rather than a single massive star collapsing on its own) which can provide the resultant BH disk system with more angular momentum, thus, a longer live, more powerful jet. Our model may also explain the presence of bright radio emission, seen in longer-lasting GRBs.

JOSEPH MCCARTY

PROGRAM: UNDERGRADUATE
SCHOOL: MASSACHUSETTS INSTITUTE OF TECHNOLOGY
GROUP: NSEC
MENTOR: FILIP RONNING
DISCIPLINE: PHYSICS
SUBJECT AREA: CONDENSED MATTER PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26745

ELECTRONIC STRUCTURE AND MAGNETIC INTERACTIONS IN *F*-ELECTRON QUANTUM MATERIALS

Interesting phenomena in *f*-electron materials include unconventional superconductivity, heavy fermion behavior, quantum spin liquid behavior, and novel critical exponents. These properties are difficult to explain from first-principles calculations due to the large difference in energy scales between the electronic structure and the magnetic exchange interactions. This project aims to calculate the electronic structure of several such materials with density functional theory, then create a simpler tight-binding model and determine the magnetic exchange interactions using perturbation theory with the *f*- and conduction-orbital hybridization. The goal is to learn if such a model can effectively explain properties of interest, in particular the novel magnetic and critical exponent behavior.

TALI NATAN

PROGRAM: POST BACHELORS
SCHOOL: KENYON COLLEGE
GROUP: P-4
MENTOR: ZHEHUI WANG (JEPH)

DISCIPLINE: PHYSICS
SUBJECT AREA: ACOUSTIC LEVITATION
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26736

INVESTIGATION OF TWO-AXIS PHASED ARRAY ACOUSTIC LEVITATOR PROTOTYPE

Acoustic levitation allows for the containerless manipulation of samples limited by density, size, and shape. For use in analysis methods, the stability of a levitated sample is paramount. Where single-axis levitators can only constrain a sample along one axis, a two-axis levitator can provide horizontal as well as vertical support. We investigate the ability of a two-axis levitator which employs phased arrays of transducers and operates at 40 kHz. This design and its accompanying “traps” (stable local pressure minima) were validated by models produced with the python toolbox Levitate. We tested the stability of water droplets and investigated the voltage required to levitate various samples for the two-axis levitator and its traps against a single-axis acoustic levitator.

JACK NATION

PROGRAM: UNDERGRADUATE
SCHOOL: NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY
GROUP: T-1
MENTOR: MARK ZAMMIT

DISCIPLINE: PHYSICS
SUBJECT AREA: ATOM PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27040

INVESTIGATION OF THE ATOMIC PHYSICS UTILIZED IN THE CALCULATION OF AIR OPACITIES

Radiation hydrodynamic simulations are utilized to model a range of programmatic and research applications/scenarios in order to detect, model and characterize physical objects and phenomena, such as meteoroids or vehicle (re)entry, fireballs, etc. One of the key inputs of these simulations is the Rosseland mean opacity. In order to explore the accuracy of the Rosseland mean opacity, we have investigated the uncertainty of the opacity calculations with respect to the atomic physics approximations utilized. Here we used the Los Alamos suite of atomic physics codes to calculate the Rosseland mean opacity of N and O for low-temperature air plasma modeling. Results from this investigation will help inform complete atmospheric air opacity calculations that will include molecular contributions.

LE NGUYEN

PROGRAM: GRADUATE
SCHOOL: ROCHESTER INSTITUTE OF TECHNOLOGY
GROUP: XCP-8
MENTOR: DEREK ARMSTRONG
DISCIPLINE: PHYSICS
SUBJECT AREA: COMPUTATIONAL PHYSICS
TYPE: INDIVIDUAL

LA-UR-22-26028

NEURAL NETWORKS FOR NEUTRON AND PHOTON TRANSPORT INTERPOLATION

Los Alamos National Laboratory (LANL) simulates low altitude (< 10 - 15 km) and ground based EMP (Electromagnetic Pulse) with Monte Carlo N-Particle (MCNP) and Finite Difference Time Domain (FDTD) codes. These models are extremely computationally expensive, taking on the order of weeks to run using multiple nodes on LANL's high performance computing platforms. The majority of the run-time is in MCNP calculating the energy deposition rate and photocurrent density to feed into FDTD which calculates the EMP's electric field. The immense amount of computational time taken hinders LANL's EMP research and this project seeks to cut down on computational expense by using neural networks as a surrogate model for MCNP.

VIA NIELSON

PROGRAM: UNDERGRADUATE
SCHOOL: UNIVERSITY OF MICHIGAN
GROUP: MPA-Q
MENTOR: MALCOLM BOSHIER

DISCIPLINE: PHYSICS
SUBJECT AREA: CQUANTUM PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26728

NUMERICAL SIMULATION OF AN ATOM INTERFEROMETER

We are writing a python package to simulate an atom interferometer (AI). The AI is described by a nonlinear Schrodinger equation known as the Gross-Pitaevskii equation (GPE). We solve the GPE numerically for the dynamics of the Bose-Einstein Condensate (BEC) used in the AI. The AI realizes a rotation sensor by splitting the BEC into wavepackets that move in opposite directions around a loop. Rotation changes the phase difference between the wavepackets when they meet. The loop area is made as large as possible to increase sensitivity. Numerical simulation on a mesh covering a large loop area is made possible by representing the wavepackets as plane waves multiplied by an envelope that varies slowly in space and time. A split-operator method is used to propagate the envelope wavefunctions.

RYAN PARK

PROGRAM: POST BACHELORS
GROUP: T-1
MENTOR: MARK ZAMMIT
DISCIPLINE: PHYSICS
SUBJECT AREA: ELECTRON SCATTERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26187

A GENERAL ANALYTIC ELECTRON ENERGY SHARING MODEL FOR MONTE-CARLO PLASMA CODES

Modeling non-equilibrium plasmas with Monte Carlo collision codes or Boltzmann equation solver codes requires input of collision cross sections and or scattering models. Recently we have developed a general analytic scattering model for calculating the electron-impact ionization electron energy sharing distribution (EESD) function, which can be readily implemented in Monte Carlo simulation codes. We present our model with a wide range of impact energies, species, ions, and species excited states and compare our approach to scattering models generally used by collisional Monte Carlo codes, e.g., the EESD of C. B. Opal et al. J. Chem. Phys. 55, 4100 (1971), the equal-energy sharing approximation, and approximating the primary electron to take all excess energy.

Andres Pruet

PROGRAM: POST BACHELORS
SCHOOL: NEW MEXICO INSTITUTE OF MINING & TECHNOLOGY
GROUP: WRS-WMT
MENTOR: JULIE MAZE
DISCIPLINE: PHYSICS
SUBJECT AREA: PARTICLE PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-25876

MIE SCATTERING DATA ANALYSIS

This summer I was tasked with analyzing Mie Scattering data and ingesting the data into the National Security Data Solution repository (NSDS).

CHRISTOPHER ROPER

PROGRAM: GRADUATE
SCHOOL: GEORGIA INSTITUTE OF TECHNOLOGY
GROUP: ISR
MENTOR: QUINN MARKSTEINER
DISCIPLINE: PHYSICS
SUBJECT AREA: APPLIED PHYSICS PLASMA PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-25656

BEAM PLASMA INTERACTIONS EXPERIMENT: USING A SPACE-BASED ACCELERATOR SYSTEM

Electron beam experiments have been used to study spacecraft-plasma coupling, spacecraft charging, and wave generation in the past. Recently, new advances in space technology, diagnostics, and accelerators have enabled a paradigm shift for a new generation of active space experiments using electron beams. This shift opens an opportunity to expand knowledge of wave and wave-particle interactions, a critical role in some of the most important dynamics in space and astrophysical plasmas. This research effort, we present progress on The Beam Plasma Interactions Experiment (Beam-PIE): a sounding rocket experiment that will use an electron beam to quantitatively understand and characterize how energetic electron beams in space couple to plasmas to stimulate whistler-mode and R-X-mode radiation.

ENRIQUE SEGURA CARRILLO

PROGRAM: GRADUATE
SCHOOL: CU BOULDER
GROUP: MPA-Q
MENTOR: MICHAEL MARTIN

DISCIPLINE: PHYSICS
SUBJECT AREA: QUANTUM INFORMATION SCIENCE
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-27125

DEVELOPING BLUE-DETUNED OPTICAL BOTTLE BEAMS FOR COLD RYDBERG ATOM TECHNOLOGIES

Cold Rydberg atom arrays are systems suited for scalable quantum simulation, computation, and sensing. These applications require robust manipulation of atomic quantum states. Blue-detuned optical Bottle Beams (BOBs) create a tightly confining 3D trap in which cold atoms will be trapped and localized. BOBs are unique because they trap an atom at an intensity minimum, thus minimizing atomic heating, decoherence rates, and light shifts. These favorable properties make BOBs ideal for coherent quantum control. We create arrays of BOBs by imprinting a phase mask on an incoming beam with a spatial light modulator and propagating this beam through an objective lens, yielding a micron-sized trap array. Creating an array of trapped atomic qubits enables a host of quantum engineering applications.

CELIA TORAL

PROGRAM: UNDERGRADUATE
SCHOOL: CORNELL UNIVERSITY
GROUP: T-3
MENTOR: ROSEANNE CHENG
DISCIPLINE: PHYSICS
SUBJECT AREA: HIGH-TEMPERATURE SHOCK PHYSICS
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26826

HYDRODYNAMIC MODELING OF THE TAYLOR-VON NEUMANN-SEDOV BLAST WAVE

Computational hydrodyamics is an essential skill set for a wide range of LANL initiatives. In this project, principles of fluid mechanics and high performance computing are merged through the ATHENA++ hydrodynamics code to solve the Taylor-von Neumann-Sedov blast wave problem. The governing equations are the conservation laws of mass, momentum, and energy and the ideal gas equation of state. In addition to HPC, we derive self-similar solutions to solve this set of equations. Making the comparison between our numerical and self-similar solutions is an excellent test of ATHENA++. The ultimate goal of this work is to apply ATHENA++ to new applications ranging from problems in national security to astrophysical phenomena such as the propagation of supernovae remnants.

LEO TUNKLE

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SUBJECT AREA: NUCLEAR ENGINEERING
TYPE: INDIVIDUAL PRESENTATION

LA-UR-22-26348

IMPROVING GROUP STRUCTURE CHOICES FOR NEUTRONICS APPLICATIONS

Deterministic neutron transport codes require discretization of the energy domain into energy groups. Simulation speed and accuracy are each affected by the choice of group structure. This project seeks to find group structures that work well for various neutron criticality benchmarks and potentially provide reasoning for why they work well. For this purpose, thousands of simulations will be run using the PARTISN deterministic transport code on various criticality benchmark problems. These will use thousands of random 30 group structures chosen from the LANL-618 group structure and results will be compared to output using the LANL-30 group structure as well as to experimental data.

ISAIAH WALL

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LA-UR-22-26811

NOVEL APPROACH TO MEASURING ACETONE CONCENTRATION FOR APPLICATIONS IN PLIF

Measuring the concentration of acetone for Planar Laser Induced Fluorescence (PLIF) is a persistent problem in the experimental community. For quantitative concentration measurements to be calculated from PLIF data, the initial concentration of acetone (usually mixed with air or nitrogen) is necessary. Lack of dedicated equipment designed to measure this value makes monitoring this value in real time during an experiment challenging. This project aims to create a small, affordable device to measure concentration by applying the Beer-Lambert's law to a small volume of an acetone mixture. More accurate readings of acetone concentration can be used to improve experimental data and further understanding of fluid phenomena.

XIAOHAN WAN

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LA-UR-22-26018

TOPOLOGICAL FLAT BAND IN BUCKLED MONOLAYER GRAPHENE

The buckling of two-dimensional materials provides a strategy to stabilize novel quantum states by creating superlattice systems. Recently it was shown by experiment that buckled graphene superlattices can have flat electronic bands. In this project, we study the topological states in the buckled graphene. We develop theory to understand the effects of the pseudo magnetic field introduced by buckling on Dirac fermions. The buckling stabilizes both the topologically trivial and nontrivial flat band through strain. The flat band sets a stage for emergence of strongly correlated quantum state, which will also be investigated.

NOSHEEN YOUNAS

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SUBJECT AREA: PHYSICS/PHYSICAL CHEMISTRY
TYPE: INDIVIDUAL PRESENTATION
LA-UR-22-26957

MODE PROJECTION FOR DIMENSIONALITY REDUCTION IN OPEN QUANTUM SYSTEM DYNAMICS

Creation and manipulation of quantum states is of paramount importance in applications such as quantum computing. In any given physical realization of the quantum states, the states of interest interact with the environment. Tracking the effects of these interactions often becomes computationally infeasible due to extremely large size of the environment degrees of freedom. Multiple techniques have been invented to tackle this challenge. One such method is Singular Value Decomposition (SVD), which can reduce the environment degrees of freedom by generating a handful of computationally relevant modes. This project applies SVD on an environment of phonons that interact with the spin states of metallic ions in metal organic frameworks.