LOS ALAMOS NATIONAL LABORATORY

2023 Student Symposium Project Description Book

The Student Programs Office

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Biological Science

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Program: Graduate Student
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Group: B-GEN
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Discipline: Biological Science
Subject Area: Microbiology
LA-UR-23-27463

CHASING AFTER ANCIENT BACTERIA RELEASED FROM THAWING PERMAFROST DUE TO CLIMATE CHANGE

Permafrost is a reservoir for ancient microorganisms that have been frozen for tens or thousands of years. Recent evidence has shown that wildlife and human populations have been impacted. While permafrost is likely to harbor “novel” microbes that have not seen a plant, animal, or human host for thousands of years, the possibility of a pathogenic threat on a pandemic scale exists. Thus, it is critical to actively biosurveille thawing permafrost to characterize the ancient microbes being released to the modern environment and through genomics, assess any threats they may pose to our public health, environmental, and national security. The goal of this project is to develop LANL’s unique capabilities of single cell genomics and gel microdroplets to a more streamlined mode to improve cultivation and genomic characterization of novel bacteria. My work will be applied on Alaska permafrost that exhibit two degrees of thaw: most disturbed (MD) and undisturbed (UD).

Grace Leito

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Group: A-1
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Discipline: Biological Science
Subject Area: Environmental Epidemiology
LA-UR-23-27798

UNDERSTANDING THE CONTROLS OF CLIMATE ON VALLEY FEVER INCIDENCE IN ARIZONA

Valley fever, also named coccidioidomycosis, is a fungal disease endemic in the southwestern portion of the United States. Once people breathe the spores of the fungus in, an infection of the lungs can occur, leading to debilitating symptoms and even death. Valley fever endemicity is largely influenced by climate conditions that promote the growth and dispersal of the Coccidioides fungus. The climate that it thrives in are areas that experience heavy rainfall followed by periods of drought. As climate changes, the conditions suitable for Coccidioides are expected to change and so far, there isn't a method to forecast Valley fever cases in relation to the climate. In this study, we analyze previous climate conditions and disease incidence data from 2000 to 2019 in Arizona, one of the highest endemic regions. We analyzed soil moisture, precipitation, and temperature, based on biological hypotheses from literature review and correlation analysis. Creating a forecast model for Valley fever is needed to fully anticipate, prepare, and prevent cases, especially in response to climate change.

Aditi Lohar

Program: Undergraduate Student
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Discipline: Biological Science
Subject Area: Biological Science
LA-UR-23-28234

INVESTIGATING HAP AS A VACCINE ANTIGEN FOR NON-TYPEABLE HAEMOPHILUS INFLUENZAE

Haemophilus influenzae (Hi) is a pathogenic bacterium that causes invasive diseases such as pneumonia and meningitis in children and adults. The encapsulated form of Hi is known as Hib, and the non-encapsulated form is known as non-typeable Haemophilus influenzae (NTHi). While Hib has multiple licensed vaccines with good efficacy, the NTHi vaccine has not shown promise. This possibly stems from low immunogenicity of protein D used as antigen in these vaccines. Hap protein is another potential NTHi vaccine antigen currently under investigation. Human leukocyte antigens (HLA) present protein fragments to immune cells that determines immune activity. We analyzed HLA binding affinities and immunogenicity of peptides derived from Hap. We further performed polymerase chain reaction to determine specific HLA-B alleles in three human serum samples and analyzed binding affinity and immunogenic scores for Hap protein. Our results show that Hap can be developed into a potential NTHi vaccine candidate.

Anika Lovato

Program: High School Student
School: Los Alamos High School

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Discipline: Biological Science
Subject Area: Biological Science
LA-UR-23-28231

REGIONAL COMPATIBILITY FOR PRN ANTIGEN IN BORDETELLA PERTUSSIS VACCINES

Bordetella pertussis is a coccobacilli that causes the disease "whooping cough" and is responsible for the mortality of about 160,700 infants each year. This rate is significantly increasing due to vaccine resistance and reduction in duration of immunity. Human Leukocyte Antigen (HLA) alleles were used to investigate variation in binding affinity to pertactin (PRN), a protein commonly used in B. pertussis vaccines. The 25 most frequent HLA-B alleles from a total of 11 regions and the PRN antigen sequence were entered into an immune epitope database to assess the binding affinity score between the allele and the vaccine antigen. By using binding affinity and allele frequencies we can better design vaccines to provide lasting immunity for most people.

Anna Matuszak

Program: Post-Bachelor's Student
School: New Mexico State University

Group: C-PCS
Mentor: Jessica Kubicek-Sutherland
Discipline: Biological Science
Subject Area: Biological Science
LA-UR-23-28233

POTENTIAL VACCINE ANTIGEN FOR B. ANTHRACIS

Bacillus anthracis, the pathogen that causes the disease anthrax, is considered a Category A Biothreat due to its ability to be synthetically manufactured and aerosolized through spores. This necessitates a reliable vaccine to protect against a possible outbreak. The protective antigen (PA) on B. anthracis serves as a potential vaccine component. Human Leukocyte Antigens (HLA) recognize foreign molecules in the human body and trigger an immune response by presenting the peptide to T-cells. Polymerase chain reaction (PCR) was performed to evaluate which HLA-B alleles are represented in different human samples. The binding affinity and immunogenicity of the PA and HLA alleles were evaluated to see how well a vaccine could stimulate antibody production. HLA-B*58:01 is a very common HLA allele worldwide and showed a high binding affinity to the PA sequence. This binding affinity analysis can be used to investigate variation in vaccine efficacy across different regions of the world.

Hanna Mora

Program: Undergraduate Student
School: New Mexico Highlands University

Group: EPC-ES
Mentor: Jenna Stanek
Discipline: Biological Science
Subject Area: Wildlife Biology and Conservation
LA-UR-23-26926

WESTERN BUMBLEBEE SURVEYS ON LANL

Bombus occidentalis commonly known as the Western Bumblebee is petitioned to be listed under the Endangered Species Act due to their significant decrease in population size. The Western Bumblebee can be found along the Pacific Coast and into the western interior of North America, including New Mexico. Prior to 1998 the Western Bumblebee's range was widespread into the western United States and Canada. Since 1998 the bee has seen a drastic decline in population and observance throughout its previous ranges including, New Mexico. Conducting surveys for the Western Bumblebee is important as it not only helps the laboratory maintain the proper procedures should the species be federally listed under the Endangered Species Act, but it also keeps accountable all the other species of bumblebees that reside on or around LANL property and allows us to be better environmental stewards and protect the bumblebees and their habitats.

Sarah Mozden

Program: Post-Bachelor's Student
School: Rice University

Group: B-TEK
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Discipline: Biological Science
Subject Area: Biotechnology

LA-UR-23-27587

CASCADE AMPLIFICATION BIOLOGICAL SENSORS FOR NOVEL ANTIBODY-BASED DETECTION ASSAY

Detection platforms based on PCR are sensitive and specific but are slow and require specialized instrumentation. Traditional Lateral Flow Assays are simplistic and quick but have lower sensitivity thresholds. We aim to create a biothreat detection platform that is both simplistic and has high sensitivity. CABS, our novel detection platform, uses a cascade of antibodies and hinges on LANL-developed split fluorescent proteins (FPs). First, two antibodies with non-overlapping recognition sites bind to a target protein, reconstituting a split green FP (GFP). Next, this GFP is recognized by a pair of nanobodies whose tails reconstitute a split red FP (RFP), causing signal amplification. CABS requires a mixture of nanobodies specific to fluorescent proteins and the components required for tripartite RFP/GFP to create this cascade amplification system, which is faster and demonstrates higher specificity than current technologies. Data on developing antibodies, nanobodies and split fluorescent proteins will be displayed and presented.

Erika Quezada Alcantar

Program: Post-Bachelor's Student
School: Northern New Mexico College

Group: B-IOME
Mentor: Claire Sanders

Discipline: Biological Science
Subject Area: Biofuels
LA-UR-23-27320

NUTRIENT UPTAKE AND BIOMASS PRODUCTIVITY IN MICROALGAE

Microalgae are a promising source for biofuels and bioproducts; however, production costs need to be reduced, and productivity increased, to make them competitive. We studied the effect of varying the media concentrations of essential macronutrients on algae growth, nitrogen and phosphorus on biomass productivity. We chose two highly productive algal strains, Picochlorum celeri and Tetraselmis striata to grow in environmental photobioreactors, which simulate outdoor light and temperature conditions. We tested various nutrient conditions, 20-140 ppm N and 2-19 ppm P, and examined differences in growth to determine which nutrient combination yielded maximum productivity, and lowest production costs. In conjunction with collaborators, we tested a subset of these conditions in outdoor raceway ponds. Our results show that the tested conditions did not have a significant impact on algae biomass productivity, indicating their robustness to nutrient variations. Techno-economic analysis shows that reducing nutrient inputs significantly lowers the cost of biomass production.

Makenzie Quintana

Program: Post-Bachelor's Student
School: New Mexico State University

Group: EPC-ES
Mentor: Elisa Abeyta
Discipline: Biological Science
Subject Area: Wildlife Biology
LA-UR-23-27672

EVALUATION OF A NOVEL CAMERA TRAPPING METHOD FOR SMALL MAMMALS

An array of trapping methods have been developed to monitor and capture small mammals for assessment. Some trapping methods, such as Sherman traps, require handling, which could stress or injure an animal. We sought to evaluate the Hunt trap, a non-invasive alternative trapping method for small mammals, which are often difficult to detect with conventional camera trap surveys. The modified Hunt trap design was made of a 7-gallon bucket with grid paper attached to the bottom, PCV pipe fastened to hold the bait, two openings on the side, and a game camera mounted on the lid facing down. We deployed four traps at Los Alamos National Laboratory, in ponderosa pine forest. Preliminary results detected harvest mice (Reithrodontomys), deer mice (Peromyscus), wood rats (Neotoma), rock squirrels (Otospermophilus) and chipmunks (Neotamias) at the Hunt trap. The results from the Hunt trap method will be compared to prior Sherman trap data at the same site. Our preliminary findings suggest that the Hunt trap may be useful as a non-invasive tool to survey small mammal communities.

Nelson Ruth

Program: Post-Master's Student
School: University of Oregon

Group: B-GEN
Mentor: Migun Shakya
Discipline: Biological Science
Subject Area: Bioinformatics
LA-UR-23-25846

GENOMIC CHARACTERIZATION OF MICROBIAL POPULATIONS IN UNTREATED WASTEWATER FROM AROUND THE WORLD

Wastewater is regularly used for tracking known and emerging pathogens, but its overall microbial diversity remains relatively unknown. In order to track both known and yet to be known pathogens in wastewater, we need to have a better understanding of what kind of microbes are typically found in wastewater. Here, we surveyed global untreated wastewater by analyzing 1,529 metagenomes, metatranscriptomes, and metaviromes covering 6 continents. We have recovered and characterized a large amount of high-quality bins and viral contigs, assessed the taxonomic content and overall diversity of wastewater microbiome, and recovered microbes inherent to specific locations and shared across continents. Our study provides one of the first comprehensive descriptions of untreated wastewater microbiomes.

Dana Urbatsch

Program: Undergraduate Student
School: Arizona State University

Group: B-GEN
Mentor: Shawn Starkenburg
Discipline: Biological Science
Subject Area: Microbiology
LA-UR-23-27783

STRAIN DEVELOPMENT AND CHARACTERIZATION OF PICOCHLORUM SPP. FOR IMPROVED MICROALGAL BIOMASS PRODUCTIVITY

For the production of algae to be cost competitive on a commercial scale, strains must be developed that can reach the goal of 25g m-2 day-1 for year-round production. In order to increase the productivity of algae genera of interest, certain strains can be mutated or evolved in the lab to have faster growing times. Picochlorum renovo has been identified as a strain that can withstand higher temperatures in field cultivation. Through random insertional mutagenesis, 96 different transformants can be grown and phenotyped in an efficient pipeline. This phenotyping pipeline uses miniaturized culturing techniques, lipid and starch stains respectively, and optical density and chlorophyll fluorescence in order to measure cell density and growth. The development, isolation, and then testing of altered algae strains has led to an increase in productivity compared to the wild type strains, which can be further applied to increased resilience in the field.

Kayley You Mak

Program: Graduate Student
School: University of New Mexico

Group: B-GEN
Mentor: Blake Hovde
Discipline: Biological Science
Subject Area: Biology
LA-UR-23-27016

INCREASING BACTERIAL TOLERANCE AND METABOLISM USING COMMUNITY-LEVEL EVOLUTION AND FUNCTIONAL GENOMICS OF THE BIOFUEL, N-BUTANOL

n-butanol is a strong biofuel candidate since it is more energy dense and less volatile than ethanol. The bottleneck for industrial production of n-butanol is the toxicity; most microbes cannot survive above 1.5% v/v. We propose to develop bioremediation capability along with the biofuel capacity to mitigate future spills. Two main approaches were used: community-level screening and functional genomics, both followed by directed evolution to increase biodegradation. A bacterial library from historic bioremediation projects was re-isolated, then mixed into artificial communities of ~20 strains. These strains were screened for tolerance to butanol, and continuously exposed to increase tolerance. Secondly, we looked for bacteria with alcohol dehydrogenase enzymes and looked to increase butanol metabolism. The tolerance for n-butanol may be improved with repeated exposure, but it was difficult to switch from tolerance to metabolism. Bacterial community dynamics were influenced by n-butanol concentration. More work is needed to understand the biodegradation of butanol.

Chemsitry

Shinhyo Bang

Program: Graduate Student
School: Washington State University

Group: EES-16
Mentor: Hongwu Xu
Discipline: Chemistry
Subject Area: Materials Chemistry
LA-UR-23-27834

HIGH ENERGY RESOLUTION X-RAY ABSORPTION SPECTROSCOPY STUDY OF COFFINITE UNDER VARYING PRESSURE

Uranium L3 HERFD-XANES spectra of coffinite were collected under varying pressure until 25 GPa. Systematic changes in the spectra's peak position and branching ratio were observed.

Hope Brown

Program: Graduate Student
School: University of Oregon

Group: MST-7
Mentor: Brennan Billow
Discipline: Chemistry
Subject Area: Engineered Materials
LA-UR-23-23305

SYNTHESIS AND CHARACTERIZATION OF SILICONE BASED SEGMENTED POLYURETHANE/UREAS

Segmented polyurethanes with traditional polyester soft segments are highly susceptible to hydrolysis of the backbone. Polyurethanes with silicone soft segments stand to increase the hydrolysis resistance compared to these traditional polyester soft segments due to the increased stability of Si-O linkages as compared to ester functionalities. In this study, polyurethanes made with polydimethylsiloxane (PDMS) soft segments are being investigated. We expect PDMS's retention of flexibility and increased resistance to hydrolysis to improve the stability of the polyurethane polymer while retaining the desired mechanical properties.

Gabriel Juarez

Program: Graduate Student
School: University of Texas at Austin

Group: C-IIAC
Mentor: Tondreau, Aaron Tondreau
Discipline: Chemistry
Subject Area: Inorganic and Organometallic Chemistry
LA-UR-23-28104

SIMPLE-CHELATES, CRYPTANDS AND EXPANDED CAGES FOR THE F-ELEMENTS

An FDA-approved iron-chelator, deferasirox (ExJade), employed in the treatment of iron overload, was modified for the chelation of lanthanide ions. Due to the benzoic acid functional group of ExJade, oligomer chains formed upon complexation. Thus, two ExJade derivatives, ExPh containing a phenyl group and ExBT with a benzothiazole group, were used in this study. Single crystal x-ray diffraction (SC-XRD) crystallography was implemented to provide structural determination of the simple chelates. ExBT-La and -Eu crystals expressed dimeric structures while the ExBT-Lu crystal revealed a 7-Lu cluster. The structural difference supported the selective precipitation of ExBT-Lu at 80% in competition with La(III), Ce(III), and Eu(III) in a 1:1 mixture. These results are guiding the use of an encapsulating macrocycle: an expanded macrocyclic chelate (Tris(naphthyridine-diimine)bis[Tren]; ExTPT). This macrocycle displays size-dependent coordination of metal cation, where early-late lanthanide separations may benefit from binding differences.

Justin Ruthstorm

Program: Graduate Student
School: New Mexico Institute of Mining and Technology

Megan Manzanares

Program: Undergraduate Student
School: University of Denver

Benjamin Rhoads

Program: Graduate Student
School: University of Mississippi

Group: ORI-2
Mentor: Alexander Bishop
Discipline: Chemistry
Subject Area: Machine Learning
LA-UR-23-27970

UNSUPERVISED DETECTION OF CORROSION ON NUCLEAR MATERIAL STORAGE CONTAINERS

Surveillance of nuclear material storage containers is currently operated using human-intensive efforts. These efforts can lead to a high radiation dose from materials stored within said containers. The SAVY-4000 is Los Alamos National Laboratory's Manual 441.1-1 compliant storage container of choice, which is constructed with 316L stainless steel. The filter on the lid is our best insight regarding the degree of corrosion that may be occurring inside the container. By submitting thousands of pristine SAVY-4000 container pictures to the machine learning model PaDiM, the network is trained to recognize anomalies such as corrosion. The threshold for determining whether there is an anomaly is tuned to minimize the number of missed anomalies and improve overall accuracy. It is found that PaDiM can recognize anomalies with an accuracy of 96.6% as well as pristine images with an accuracy of 89.2%. These efforts hope to prevent exposure by nuclear radiation inside the facility.

Jacob Mitchell

Program: Graduate Research Assistant
School: University of Oregon

Group: MST-7
Mentor: Amanda Graff
Discipline: Chemistry
Subject Area: Polymer Science
LA-UR-23-27607

FABRICATION OF QUANTUM DOT SOLID-STATE DETECTORS

Detection methods for γ-radiation employ commercial solid-state detectors containing high purity germanium (HPGe) and cadmium zinc telluride (CZT) as sensing materials. However, the drawbacks of HPGe (which requires cryogenic operating temperatures) and CZT (which involves the growth of impurities) limit their utility in operational environments, but also motivate the development of new solid-state detectors. Quantum dots have shown the ability to interact with γ-radiation, and their unique ability to alter the optoelectrical properties with size makes them a prime candidate for new solid-state detectors. We propose a novel and safe method for synthesizing near monodisperse cadmium selenide QDs using flow chemistry. Subsequently our group aims to fabricate working solid-state detectors utilizing a cadmium selenide/ poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV) bulk heterojunction morphology (BHJ). Correspondingly our group will study the effects of QD size and surface chemistry on the efficiency of these new generation solid-state detectors.

Victoria Nisoli

Program: Undergraduate Student
School: University of New Mexico

Group: MPA-CINT
Mentor: Jennifer Hollingsworth
Discipline: Chemistry
Subject Area: Nanotechnology
LA-UR-23-27966

NEAR-INFRARED PLASMONIC PROPERTIES IN SPINEL METAL OXIDE NANOMATERIALS

Nanomaterials with optical properties capable of reaching the telecommunications region (~1300-1550 nm) are of increasing interest due to their applications in light-based communication. Quantum emitters, like quantum dots (QDs), are capable of emission in this infrared (IR) wavelength range, but they can produce photons too slowly. For fast emission, QDs can be combined with materials capable of supporting a localized surface plasmonic resonance (LSPR) that acts to make QD emission faster. The LSPR needs to overlap with the wavelength of the QD emission. Here, we demonstrate the ability to synthesize spinel plasmonic nanomaterials that have LSPR wavelengths in the telecom window. In particular, we synthesize high-quality nanocrystal cubes that can be used to construct a special type of plasmonic antenna, known as a nanogap antenna. We show how an emitter placed in the gap experiences a particularly strong plasmonic effect and becomes an ultrafast emitter.

Renee Olney

Program: Graduate Student
School: University of Nevada, Las Vegas

Group: C-NR
Mentor: Jeremy Inglis
Discipline: Chemistry
Subject Area: Radiochemistry
LA-UR-23-27148

NOVEL METHOD FOR URANIUM HEXAFLUORIDE ISOTOPE RATIO MEASUREMENT

Examination of an alternative method for the collection, transportation, and analysis of uranium hexafluoride for nuclear safeguards using room temperature ionic liquid.

Osvaldo Ordonez

Program: Graduate Student
School: University of California, Santa Barbara

Group: C-IIAC
Mentor: Andrew Gaunt
Discipline: Chemistry
Subject Area: Actinide Chemistry
LA-UR-23-27582

EXPANDING METAL LIGAND MULTIPLE BONDS IN NEPTUNIUM

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 specialized 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.

Marina S. Pacheco Davil

Program: Post-Bachelor's Student
School: University of Texas Rio Grande Valley

Group: MPA-11
Mentor: Eun Joo (Sarah) Park
Discipline: Chemistry
Subject Area: Chemistry
LA-UR-23-27821

DEVELOPMENT OF REINFORCED ION EXCHANGE MEMBRANES

Hydrogen, the cleanest source of renewable energy, is now readily available by technologies such as water electrolysis, the process of splitting water into hydrogen and oxygen. Membrane driven water electrolysis is a promising technology that can produce pressurized hydrogen with high production efficiency. Ion-exchange membranes (IEMs) are critical in membrane-based applications by transporting oppositely charged ions and consist of polymers with ionic groups attached to the backbone. IEMs face a mechanical durability issue, for which the implementation membrane support materials and cross-linking are promising solutions. In this research, reinforced anion-exchange membranes (AEMs) were fabricated using a porous substrate, with polymerizing and in-situ cross-linking of 4-vinylbenzyl chloride. The membranes were quarternized to produce anion exchanging trimethyl ammonium groups. The reinforced AEMs were characterized and evaluated for membrane properties in comparison to free-standing membranes. This approach can be applied to other vinyl monomers synthesized, producing sulfonated hydrocarbon proton-exchange membranes with mechanical enhancement.

Hannah Patenaude

Program: Graduate Student
School: University of Nevada, Las Vegas

Group: C-IICA
Mentor: Marisa Monreal
Discipline: Chemistry
Subject Area: Actinide Molten Salt Chemistry
LA-UR-23-26740

ELECTRODE MATERIALS FOR F-BLOCK ELECTROANALYTICAL CHEMISTRY IN MOLTEN CHLORIDE SALTS

As the reality of operating commercial Molten Salt Reactors (MSRs) draws nearer, there is still a need for fundamental research on fuel salt systems. However, molten salt experiments are particularly challenging given the high temperature, corrosivity, and radioactivity of these systems. This study compares the results of voltammetric techniques using working electrodes fabricated from tungsten, graphite, and boron-doped diamond (BDD) to study various f-block elements in molten chloride salts. Ultimately, the BDD electrode produced the highest resolution oxidation and reduction peaks. While materials like tungsten and graphite have successfully measured redox couples in molten salts previously, the BDD electrode performance was superior to these metal and non-diamond carbon options. BDD will be further explored through various materials characterization pathways to better understand its resilience in molten salts. Additionally, it will be applied to studies of other analytes relevant to MSR fuels, including other f-block elements.

Jason Ross

Program: Post-Master's Student
School: University of Missouri

Group: MPA-11
Mentor: George Goff
Discipline: Chemistry
Subject Area: Inorganic Chemistry
LA-UR-23-27688

SYNTHESIS OF NOVEL LANTHANIDE TASK SPECIFIC IONIC LIQUID COMPLEX'S UTILIZING BETAINE TRIFLATE

Within the United States there lacks an efficient way to purify lanthanide metals in an environmentally friendly and efficient way. To provide a solution for difficult separation methods, judicious selection of a material is needed. Ionic liquids serve as a answer because of their negligible vapor pressure, high thermal stability, and tunable properties. The development of a novel ionic liquid that exhibits lanthanide metal chelation can be utilized to isolate, and purify, lanthanide metals without impacting the surrounding environment. Within this work, the overall goal is understanding complex interactions of lanthanides and their interactions with a novel ionic liquid to improve lanthanide separation schemes. Techniques involving UV-Vis and single crystal x-ray diffraction are utilized to elucidate speciation and solid-state structures, respectively. Current results demonstrate that neodymium and samarium form dimeric compounds whose structure mimic those previously reported but vary in lattice packing. Exploration across the lanthanide series is currently underway.

Matthew Salinas

Program: Undergraduate Student
School: University of Texas Rio Grande Valley

Group: MPA-11
Mentor: Daniel Leonard
Discipline: Chemistry
Subject Area: Electrochemistry
LA-UR-23-27968

IONIC CONDUCTIVITIES OF ZIRFON AND POLY(BENZIMIDAZOLE) POLYMERS IN POTASSIUM HYDROXIDE ELECTROLYTE

Clean energy research has turned to the development of carbon-free production methods for hydrogen gas to harness its potential in an environmentally sustainable manner. Of these methods, alkaline water electrolysis (AWE), an electrochemical process in which water is split into hydrogen and oxygen gas, is attractive due to its technological maturity and low capital requirements. However, an impediment to the increased use of AWE is its low energy efficiency and hydrogen production rate, due in part to the unsatisfactory conductivity of the involved ion-solvating polymer (ISP) separators. The role of these separators is to allow ions to be conducted across the cell while still preventing short-circuiting and unsafe mixing of the gaseous products. Poly(benzimidazole) (PBI) shows promise not only as a selective membrane but as an effective ionic conductor. This project aims to quantify and compare the conductivity exhibited by PBI to that exhibited by the industry-standard separator, Zirfon.

Cameron Taylor

Program: Graduate Student
School: Texas A&M University

Group: B-IOME
Mentor: Nilusha Subasinghe
Discipline: Chemistry
Subject Area: Organic Chemistry
LA-UR-23-27291

BIODEGRADABLE CHEMICAL HERDERS FOR OIL SPILL REMEDIATION

Oil spills are an ever-growing threat as the world's demand for oil continues to increase, requiring more maritime transportation and drilling. One methodology of remediating oil spills is the use of in-situ burning (ISB), providing an efficient and rapid means of removing surface oil. One significant drawback for ISB is the rapid spreading of the surface oil, which inhibits the use of ISB if the slick is too thin. To avoid this issue an amphiphilic molecule called a chemical herder can be deployed in the water near a spill surround the slick. The chemical herder acts as a surfactant at the water-oil interface by utilizing the difference in surface tension to push against the oil to thicken the slick to burn (≥3 mm). Currently utilized EPA-approved chemical herders, however, pose a toxic threat to aquatic organisms. This project aims to synthesize biodegradable chemical herders utilizing phytol as the non-polar group and a variety of non-toxic polar head groups (e.g., glucose, glycerol, etc.). These newly developed chemical herders will be characterized by their spreading pressure, herding efficiency, and biodegradability to determine their oil herding efficacy in different sea water environments.

Grace Xie

Program: Undergraduate Student
School: Lake Forest College

Group: ALDWP-TAO
Mentor: David Olivas
Discipline: Chemistry
Subject Area: Data Analysis of Plutonium Isotopic Levels
LA-UR-23-27941

INVESTIGATING PLUTONIUM ISOTOPIC LEVELS

This project focuses on conducting an extensive investigation of plutonium isotopic levels obtained from various sites, namely the Chalk River, Hanford, and Savannah River Site, the Rocky Flats Plant, and the Los Alamos National Laboratory. The study encompasses three primary objectives: nuclear forensics, setting standards, and the foundational stockpile of plutonium in the United States. Through an analysis of the isotopic composition of plutonium samples, valuable information can be derived regarding their production history, reactor type, and irradiation duration, enabling source attribution. The project involves data collection and conditioning, statistical analysis, and the formation of scatter plots to uncover patterns and contribute to the understanding of plutonium isotopic levels and their implications for various applications. The investigation indicated differences between sites in certain isotopic levels, indicating that future research may yield even more significant results.

Rigobert Ybarra Jr.

Program: Graduate Student
School: University of Texas Rio Grande Valley

Group: MPA-11
Mentor: Daniel P. Leonard
Discipline: Chemistry
Subject Area: Materials Synthesis
LA-UR-23-27789

ENHANCEMENT OF NI-FOAM FOR LIQUID ALKALINE WATER ELECTROLYSIS

Hydrogen is used as a reactant in many different processes such as refining metal, energy production, and in chemical synthesis. The use of fossil fuels to produce hydrogen is the dominant method currently used adding to the problem of increasing greenhouse gases. A more sustainable production method is needed in order to simultaneously meet hydrogen demand and reduce the greenhouse gas emissions. Liquid alkaline water electrolysis (LAWE) is the most mature technologies on the market but needs significant development to both increase efficiencies and allow for compatibility with renewable energy sources. This project investigates two surface deposition techniques (electrodeposition and sputtering) on nickel electrodes to increase performance and durability of LAWE systems.

Computing and Information Technology

Andy Cox

Program: Graduate Student
School: Texas A&M University

Group: CCS-3
Mentor: Ayan Biswas
Discipline: Computing and Information Technology
Subject Area: Machine Learning
LA-UR-23-27559

EXPLORING CUNUMERIC SPEEDUP FOR IN SITU MACHINE LEARNING

Training CNN in situ with cuNumeric also testing out various kernels for training data generation.

Vivian Hafener

Program: Undergraduate Student
School: Rochester Institute of Technology

Group: HPC-ENV
Mentor: Steven Senator
Discipline: Computing and Information Technology
Subject Area: High Performance Computing Scheduling
LA-UR-23-26818

SIMULATION OF CLUSTER SCHEDULING BEHAVIOR WITH DIGITAL TWINS USING SLURM LOGS AND BATSIM

The ability to accurately simulate the impact of changes to a system's scheduler configuration on the performance of a system is a capability that can guide decisions in the administration of HPC systems, provide recommendations to improve system performance, and validate the impact that proposed changes will have on a system prior to deployment. This presentation introduces a suite of tools based on a modified version of the open source BatSim simulation platform. This can be used to evaluate the scheduling performance of a system, to examine the impact of scheduling policy changes on jobs of different types, and to evaluate the impact of scheduled maintenance or other reservations on the job flow of the system. These tools use workload files generated by historical Slurm logs to evaluate the impact of such changes to a "digital twin" of the physical cluster, with an identical cluster configuration, job details, and scheduling policy. These tools are being used to inform LANL's production HPC operations and are under active development and enhancement.

Thomas Harris

Program: Graduate Student
School: University of Melbourne

Micaela Richter

Program: Graduate Student
School: Ohio State University

Group: A-1
Mentor: Sara Del Valle
Discipline: Computing and Information Technology
Subject Area: Computational Biology
LA-UR-23-27557

UNDERSTANDING RACIAL AND ETHNIC DISPARITIES IN COVID-19 OUTCOMES USING AN AGENT-BASED SIMULATION

The COVID-19 pandemic highlighted health disparities that exist between socio-demographic groups in the United States and the need for modeling approaches that can account for these complex dynamics. Specifically, differences in case incidence, mortality, and disease burden have been found across historically marginalized racial and ethnic groups, as well as differences by gender, age, and geographic regions. Agent-based models (ABMs) are computational models for simulating movements, activities and social interactions of individuals in a dynamic environment. Hence, ABMs provide a flexible framework for exploring population heterogeneity on disease spread trends. This project incorporates race and ethnicity into EpiCast, a large-scale ABM of infectious disease spread across the United States developed at LANL. We explore the mechanisms that drive health disparities among racial and ethnic groups and quantify their impact on disease outcomes. The results of this study can inform policy decisions aimed at addressing health equity in the United States.

Dylan Johnson

Program: Graduate Student
School: University of South Alabama

Group: SRO-RL
Mentor: Brian Cain
Discipline: Computing and Information Technology
Subject Area: Computer Science
LA-UR-23-28035

AUTOMATED AND GENERATIVE EXTRACTION OF SCIENTIFIC METADATA

Current metadata collection for LANL scientific and technical documents depends on human interaction to provide accurate information, including title, authors, affiliations, and article keywords. While this may be sufficient, an approach utilizing AI/ML tools has the potential to perform these tasks with greater convenience, speed, and depth. To test this, a prototype service has been developed as a new first step in the RASSTI pipeline, using GROBID to extract information directly from PDF files. External APIs are also employed to obtain extra author information, such as affiliations and ORCIDs, and large language models such as BERT to generate keywords and summarization of articles. This information, paired with user feedback and validation, will aid in metadata creation and completeness, as well as enhanced utility of LANL information systems. Furthermore, this dataset will help deploy possible new services like an article recommendation service and fine-tuned language models operating in the LANL environment.

Meghanto Majumder

Program: Graduate Student
School: University of Oregon

Group: CCS-3
Mentor: Li-Ta Lo
Discipline: Computing and Information Technology
Subject Area: Scientific Visualization
LA-UR-23-28106

EXPLORING DATA-DRIVEN SAMPLING STRATEGIES FOR VECTOR FIELDS

Data-driven in situ data reduction potentially enables post hoc data visualization, reconstruction, and exploration with the goal of minimal information loss. Sophisticated sampling methods provide a fast approximation to the data that can be used as a preview to the simulation output without the need for full data reconstruction. Given a spatial location, data-driven sampling approaches take into account its local properties (such as scalar value, local smoothness) to determine its importance. However, no such techniques are available for vector field data, where the 3 vector components need to be considered together, not as individual scalar fields. We aim to create new sampling strategies that correctly assigns importance values to vector field locations and are effectively able to sample them. We consider various metrics to judge the efficacy of our algorithms.

Alexander Moon

Program: Undergraduate Student
School: University of Wisconsin-Madison

Gilbert Hart

Program: Undergraduate Student
School: University of Wyoming

Group: XPC-DO
Mentor: Nikolaus Cordes

Discipline: Computing and Information Technology
Subject Area: Image Processing
LA-UR-23-27334

PARALLEL IMPLEMENTATION OF A NONLINEAR DIFFUSION FILTER

Nonlinear diffusion filters are important image processing tools for reducing noise while preserving (and enhancing) edges in nondestructive X-ray tomography. These tools allow for semi-automated processing of 2D, 3D, and 4D images. Current commercially available nonlinear diffusion tools are typically single-threaded implementations on the CPU and limit input size to 2 GB. However, these filters are highly parallelizable and a GPU implementation of the filter can speed up computation and allow for processing of images larger than 2 GB. These characteristics are highly valuable when processing X-ray computed tomograms, as the high spatial and temporal resolution images generated from this nondestructive 3D imaging technique often result in raw data that can exceed 100 GB. In the presented work, we implement Weickert et al.'s Additive Operator Splitting (AOS) algorithm on Nvidia GPUs using the CUDA dialect of C++ through the PyCUDA python library. The massive parallelization of the GPU as well as the removal of the arbitrary file size restriction results in significant speedup of the AOS algorithm compared to commercially available tools.

Alexander Most

Program: Graduate Student
School: Montana State University

Group: A-4
Mentor: Nigel Lawrence
Discipline: Computing and Information Technology
Subject Area: Cybersecurity
LA-UR-23-28221

POISSON CANONICAL POLYADIC TENSOR DECOMPOSITION FOR ELECTRICAL GRID ANOMALY DETECTION

We are applying tensor decomposition to power grid data for anomaly detection. Tensor decomposition allows us to retain the multidimensional nature of the data and detect anomalies across those different dimensions better than a dimensionality reduction method like principal component analysis. This is designed to detect malicious behavior in the system.

Neel Patel

Program: Graduate Student
School: University of Kansas

Group: CCS-7
Mentor: Jered Trujillo
Discipline: Computing and Information Technology
Subject Area: Computer Architecture
LA-UR-23-27641

DEVELOPING FUTURE MEMORY SYSTEMS FOR COMPLEX CODES

We leverage LANL's proxy applications and hardware platforms to profile existing codes and bottlenecks in relevant kernels. The gathered data informs potential improvements to the memory subsystem that may integrate into the architecture of future HPC systems at Los Alamos. The data and insights presented show a need for sparse access acceleration within the memory hierarchy using specialized memory controllers and a hardware/software co-design approach. A methodology is presented for modeling potential architectural improvements using proxy apps combined with architectural simulation. Potential performance benefits of sparse access accelerators are presented using emulation with proxy applications.

Bethany Peña

Program: Post-Bachelor's Student
School: University of New Mexico

Group: XTD-IDA
Mentor: Lucille Fry
Discipline: Computing and Information Technology
Subject Area: Computer Science
LA-UR-23-27304

UNDER THE HOOD: IMPROVING ROBUSTNESS AND USER EXPERIENCE IN THE COMMON MODELING FRAMEWORK

The Common Modeling Framework is a software project that provides a common user interface for sharing, storing, and generating experiments that can be run as EAP, LAP, and SAP physics simulations. By enabling knowledge sharing and retention via a central repository, the CMF facilitates collaboration and transparency among ALDX/LANL user communities. Developers working on the CMF maintain and improve the infrastructure, ensuring that the CMF meets users' needs and continues to align with the mission of a "common,", shared framework. I will describe some of my recent development work, which includes adding support for visual documentation of experiments using HTML and refactoring our infrastructure for representing material models. Currently, I am updating and adding to our library of shared material models and extending testing capabilities. My work enhances the CMF's user experience by providing users with more tools and makes the core infrastructure more robust to future changes.

Shrey Poshiya

Program: Undergraduate Student
School: University of New Mexico

Group: CSS-3
Mentor: Diane Oyen
Discipline: Computing and Information Technology
Subject Area: Computer Science
LA-UR-23-27642

EXPLORING ROBUSTNESS BETWEEN CLASSIFICATION AND DEEP METRIC MODELS

Deep Metric Learning (DML) methods have the power to learn high-level representations of data by learning a distance function. However, like any other gradient-based model, DML models are prone to adversarial attacks. With DML models being used for many safety-critical applications such as face verification, successfully thwarting adversarial attacks is imperative. We find that initializing DML models with weights from robust classification models dramatically increases the performance of Deep Metric adversarial defenses. DML models are first initialized with classification models trained on adversarial examples from a range of severities, then are adversarially trained themselves. We also explore how features from these robust DML models transfer to classification based attacks on a variety of datasets.

Niteya Shah

Program: Graduate Student
School: Virginia Tech

Group: CCS-7
Mentor: Nirmal Prajapati
Discipline: Computing and Information Technology
Subject Area: Computer Science
LA-UR-23-27936

OPTIMIZING MOLECULAR DYNAMICS CODES FOR AMD GPUS

Molecular Dynamics (MD) simulations are widely used to study the behavior of complex systems at the atomic level. The advent of exascale computing with Frontier has enabled previously unattainable performance for large scale MD simulations. Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is a classical molecular dynamics code used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. Spectral Neighbor Analysis Potential (SNAP) is model for studying material science simulations for fission/fusion reactors. The calculation of the bispectrum components and the SNAP potential are implemented in LAMMPS. Previous work focused on optimizing TestSNAP (a proxy for SNAP) for Nvidia GPUs. The performance of hardware specific optimizations over Nvidia architectures does not directly translate to other GPU architectures. In this work, we optimize the performance of TestSNAP codes on AMD MI250X GPUs that power the Frontier machine. We profile TestSNAP to identify the bottlenecks and tune the code to devise architecture specific improvements for AMD GPUs. We obtain an overall performance improvement of 10% compared to default TestSNAP GPU implementation.

John Stack

Program: Graduate Student
School: University College London

Group: CCS-7
Mentor: Tyler Reddy
Discipline: Computing and Information Technology
Subject Area: Biophysics
LA-UR-23-27835

A HIGH PERFORMANCE PYTHON PIPELINE TO ANALYZE AND VERIFY AN ALL-ATOM SARS-COV2 MOLECULAR DYNAMICS TRAJECTORY

As part of the LANL LDRD Current and Emerging Biological Threats project, we are running one of the largest all-atom molecular dynamics simulations of a virion: a cryo-EM model of SARS-CoV-2 with 13,727,930 atoms, not including solvate. This gives an opportunity to calculate physical properties that cannot be ascertained experimentally. But running complex calculations on 10,000s of frames of a 13,727,930 atom model requires highly performant algorithms. By using biological and mathematical techniques, MDAnalysis and SciPy we have developed an initial Python analytical pipeline that calculates multiple physical properties at a speed of 15 seconds per frame. From this we can also confirm that the model matches experimental data throughout its trajectory, preventing us from wasting computational resources (which is important as all-atom molecular dynamics simulations run on timeframes of months and use thousands of CPU cores and 100s of GPUs).

Nigel Tan

Program: Graduate Student
School: University of Tennessee, Knoxville

Group: XCP-6
Mentor: Scott Luedtke
Discipline: Computing and Information Technology
Subject Area: High Performance Computing
LA-UR-23-27541

EFFICIENT PARTICLE TRACING FOR SCALABLE KINETIC PLASMA SIMULATION ANALYSIS

VPIC is a multi-purpose plasma physics code used extensively in modeling various fundamental science applications. In past work, we targeted the portability of VPIC across heterogeneous resources while preserving performance by deploying Kokkos as the interface to those resources (VPIC 2.0). In this project, we emphasize the impact of tracing particles for studying the movement and environment of particle subsets in large plasma systems. In this context, we use tracer particles to reduce the I/O load when collecting simulation data, allowing for rapid and targeted analysis of more extended simulations. We augmented the VPIC code for our effective particle tracer implementation, including particle annotations for post-analysis of simulations. Our annotation attaches a unique 32-bit integer TracerID to each tracer particle. We write the tracer data using HDF5 for performance and accessibility. We apply optimizations such as buffering and asynchronous execution for higher performance.

Nash Taylor

Program: Undergraduate Student
School: New Mexico State University

Group: E-3
Mentor: Craig Blackhart

Discipline: Computing and Information Technology
Subject Area: Computer Science
LA-UR-23-27224

HOW KNOWLEDGE-BASED SEARCH IS MAKING 75 YEARS OF LANL RESEARCH ACCESSIBLE AND DISCOVERABLE

The NRSC currently houses 75+ years of nuclear weapons research and development with more than 14 million holdings. While the information is being digitized, a need for accessibility and discoverability of information has become apparent. In order to satisfy this need, LANL is developing a cutting edge knowledge based search engine. While AI powered by Large Language Models (LLM) like ChatGPT are promising, there are limitations such as producing hallucinations. As an alternative, LANL is developing a knowledge based search capability, similar to how Google recently started integrating knowledge graphs into their search engine to improve results. LANL's system will feature full text ingestion, automatic metadata extraction, and natural language understanding which will enable automatic metadata generation, document categorization, and the discovery of inferred substantive content. The outcome is a cutting edge knowledge based search that will return fewer and more relevant documents and data than conventional keyword search.

Sankalpa Timilsina

Program: Graduate Student
School: Tennessee Technological University

Group: A-4
Mentor: Sina Sontowski
Discipline: Computing and Information Technology
Subject Area: Computer Networking
LA-UR-23-27464

NDN FOR ENHANCED SECURITY IN INDUSTRIAL CONTROL SYSTEMS

Industrial control systems have developed their unique communication protocols over time, such as Ether/IP and CIP. As these systems adopt Internet Protocol (IP) for global interconnectivity, they become more susceptible to malicious attacks due to their significant economic value. The use of IP, which was not initially designed with rigorous security in mind, leaves gaps in key security aspects such as access control, data integrity, and authenticity. To strengthen these systems, our project employs Named Data Networking (NDN), a promising future internet architecture that prioritizes content names over addresses. With content-centric security and robust namespace-based security, NDN addresses the shortcomings of IP-based networking. We're developing a tool that introduces NDN as a communication protocol within Ether/IP-based systems, aiming to enhance the security and efficiency of industrial control systems for a safer future.

Jessica Williams

Program: Undergraduate Student
School: Texas A&M University

Group: ISR-3
Mentor: Rory Scobie
Discipline: Computing and Information Technology
Subject Area: Computer Science
LA-UR-23-27715

EVALUATING ON-SATELLITE DATA PROCESSING

The status quo for satellite-based projects is to send raw data as telemetry and do processing on the ground. With advances in embedded systems and edge computing, there is opportunity to move some data processing to the satellite board. This could reduce the amount of telemetry, allow for faster actionable information, and enhanced security. Project goals were to demonstrate a variety of common data processing libraries, evaluate performance across different operating systems and programming languages, and compare speed to on-ground data processing. Doing data processing on the satellite presents opportunity to enhance security and deliver actionable information immediately instead of waiting for multiple ground-station passes to respond to data. It is possible to run a multitude of Python libraries on board, and their performance levels are adequate.

Nicholas Witkowski

Program: High School Student
School: Los Alamos High School

Group: MPA-11
Mentor: Milo Prisbrey
Discipline: Computing and Information Technology
Subject Area: Data Science/Computing

LA-UR-23-27657

USING DATA PREPROCESSING AND VISUALIZATION TO CREATE READABLE ACOUSTIC DATA

Data preprocessing and visualization are commonly used and often critical in the workflow of scientific analysis. Preprocessing is the procedure of transforming raw data to obtain a cleaner, reduced version that is easier to utilize in, e.g., machine learning. Visualization transforms data into human-interpretable images and graphs, which aids in decision making, task management, and more. In this work, we create a python package with a suite of preprocessing and visualization tools for spectral data, which is often noisy, difficult to decipher, and challenging to use in its raw form. We use basic, common python libraries such as pandas, numpy, and matplotlib to create our functions such that the package can be included in a wide variety of scripts without the need for complicated environment setup. The created package is now currently being used continuously by research scientists at LANL to assist with acoustic data science and analysis.

Yasuki Wu

Program: Graduate Student
School: University of Minnesota

Befikir Bogale

Program: Undergraduate Student
School: University of Tennessee, Knoxville

Group: XCP-DO
Mentor: Peter Maginot
Discipline: Computing and Information Technology
Subject Area: Computer Science
LA-UR-23-27769

ACCELERATING X-RAY TRANSPORT SIMULATIONS

X-ray transport simulations require performing “sweeps'' across a mesh of cells for many different x-ray angles of travel and photon energy groups. When solving a cell, a small dense system of equations is generated and solved. We are exploring how to use vectorization to increase the performance of this. We are also using Kokkos to use OpenMP threading on a CPU to solve multiple cells in parallel.

Chloe Zhou

Program: Graduate Student
School: Columbia Law School

Group: A-1
Mentor: Paolo Patelli
Discipline: Computing and Information Technology
Subject Area: Optimization
LA-UR-23-28020

RENEWABLE NATURAL GAS AND DECENTRALIZED PRODUCTION OF SUSTAINABLE AVIATION FUEL

The project aims to assess the viability of the decentralized or distributed production of sustainable aviation fuel (SAF). Previous studies have focused on centralized production of SAF, whereby SAF is produced from biomass in a single facility near biomass sources. With decentralized production, we decouple the conversion of biomass to SAF by first transforming biomass into renewable natural gas (RNG), an intermediary product that can be easily transported or virtually relocated. The RNG is injected into existing natural gas infrastructure. SAF producers can purchase RNG via direct purchase agreements or virtually in a system analogous to the renewable energy certificate (REC) system in the electricity market, allowing for greater flexibility in facility siting. We evaluate the economic and environmental costs of decentralized vs. centralized SAF production by modeling biomass supply and jet fuel demand, modeling facility and transportation costs, and optimizing for facility scale and location for both scenarios.

Earth and Space Sciences

Shuyu Chang

Program: Graduate Student
School: Penn State University

Group: EES-14
Mentor: Kurt Solander
Discipline: Earth and Space Sciences
Subject Area: Hydrology

LA-UR-23-27635

A DEEP-LEARNING APPROACH TO PREDICT RIVER TEMPERATURE IN ALASKA

The Arctic has warmed four times faster than the globe since 1979, which is deemed the Arctic amplification phenomenon. Fisheries in this region are thus potentially more vulnerable to water temperature regime shifts, with narrower range of preference and tolerance of temperature. However, how warming air temperature will manifest in rivers and streams and the primary driver of these changes remains poorly understood due to the lack of robust measurements combined with the complex interplay of glacial melt and permafrost thaw that controls the river temperature dynamics. To address this shortcoming, we developed a Long-short Term Memory (LSTM) model to reconstruct reliable river temperature time series over a high-latitude, data-sparse region of Alaska. With this model, we were able to (1) better our understanding regarding the major physical processes and drivers in controlling river temperature dynamics; (2) unravel the spatial-temporal patterns of river temperature regime shifts under a changing climate.

Jaehong Chung

Program: Graduate Student
School: Stanford University

Group: EES-16
Mentor: Javier E. Santos
Discipline: Earth and Space Sciences
Subject Area: Computational Geoscience
LA-UR-23-27648

GENERATING MULTIPHASE FLOW CONFIGURATIONS USING DIFFUSION MODELS

Microscale two-phase flow simulations are commonly used to quantify the efficiency of hydrogen storage sites, the volume of CO2 that could be sequestered in subsurface reservoirs, and the spread of a contaminant through aquifers. While these microscopic simulations can accurately characterize the effect of complex 3D structures that occur in nature, fluid-solid reactions and fluid-fluid interactions, they are computationally very expensive. Other hurdles arise due to multiple energy minimization points, complex pore geometries, and varying in-situ conditions. For the first time, we propose using denoising diffusion models to accurately and efficiently generate stable fluid configurations for subsurface flow. This model reduces the simulation time by more than an order of magnitude (compared to multiphase lattice-Boltzmann simulations). By efficiently generating fluid configurations based on arbitrary pore geometries, our model has not only the ability to completely revolutionize reservoir characterization in earth sciences, but also to provide a tool to investigate the source of the chaotic behavior observed in experiments.

Nicholas Ellis

Program: Graduate Student
School: University of Michigan

Group: EES-14
Mentor: Thom Rahn
Discipline: Earth and Space Sciences
Subject Area: Isotope Geochemistry
LA-UR-23-28036

HYDROGEN ISOTOPE MEASUREMENTS OF H2 AT LANL

Here we present a method for quantitatively separating diatomic hydrogen from gas mixtures for isotope ratio measurements via continuous flow isotope ratio mass spectrometry. The method utilizes a cold head trap at 25K to remove all gases by phase change except hydrogen. Purified hydrogen gas is then compressed to induce sorption onto cold (liquid nitrogen cooled) molecular sieve. Hydrogen recovery by this method is quantitative and yields purities in excess of 99%. These analytical methods will enable measurements of stable isotopic compositions of hydrogen sources relevant to national security interests. In future analytical sessions, we plan to target hydrogen produced by nuclear detonation that is preserved as gaseous inclusions in glasses (e.g. trinitite) that form during nuclear weapons testing. Ultimately, we expect such hydrogen signals to provide insight into the physical processes that fractionate hydrogen during detonation, and we will explore its use as a tool for forensic nuclear detection.

Emily Follansbee

Program: Post-Master's Student
School: Columbia University

Group: EES-14
Mentor: Manvendra Dubey
Discipline: Earth and Space Sciences
Subject Area: Environmental Science
LA-UR-23-27763

ORPHAN WELL METHANE EMISSIONS INFERRED FROM PLUME OBSERVATIONS

Fugitive methane gas from orphaned and abandoned oil and gas wells are among the largest anthropogenic methane sources in North America. Current methods for locating and identifying orphaned wells are expensive and difficult, making them prohibitive to use at national scale. Here we describe a simple and effective method for quantifying fugitive methane emissions from orphaned oil and gas wells using ground and UAS-based measurements of methane concentration and wind. This field study observes and calculates a methane leak plume at an abandoned orphan well and shows that leak rates can be determined to within +/- 50% under stable wind conditions and are accurate enough to screen and prioritize wells for plugging.

Nevil Franco

Program: Post-Master's Student
School: University of Alaska Fairbanks

Group: EES-14
Mentor: Kyle Gorkowski
Discipline: Earth and Space Sciences
Subject Area: Atmospheric Science
LA-UR-23-27765

SMOKE IMPACTS ON ATMOSPHERIC PROCESSING: AN OPTICAL ANALYSIS OF BROADBAND OFFLINE AND ONLINE INSTRUMENTS

To enhance our understanding of biomass burning aerosol on climate, we analyzed the optical properties–such as absorption--of vegetation from sub-Saharan Africa using wavelength-dependent instruments in laboratory settings. This approach aims to shed light on the complex interactions between biomass burning and changes to the optical properties. Controlled burns were conducted at Los Alamos National Laboratory in collaboration with North Carolina A&T State University as part of the African Combustion Aerosol Collaborative Intercomparison Analysis (ACACIA) project. The online instrument was a photoacoustic spectrometer (PASS and PAX). Offline collection used a Particle-Into-Liquid Sampler for wavelength-dependent analysis using a Liquid Waveguide Capillary Cell (LWCC) that captures the absorbance spectra of the aerosols across a wide wavelength range (190 to 1100 nm).

Daniel Hallack

Program: Graduate Student
School: University Notre Dame

Group: EES-16
Mentor: Jeffrey Hyman
Discipline: Earth and Space Sciences
Subject Area: Computational Earth Sciences
LA-UR-23-28032

EVOLUTION OF A MIXING FRONT LINE IN FRACTURE NETWORKS

In this work we will focus on mixing in a 3D fracture network and in particular on the evolution of mixing interfaces, which reflect the region where reactions occur. The mixing interface of a continuous solute injection reflects the interaction of very basic processes, such as molecular diffusion, hydrodynamic dispersion and advection. The highly heterogeneous flow systems that emerge in 3D discrete fracture networks makes this interface behavior a highly dynamic nonlinear process. Using Los Alamos National Lab's dfnWorks model, we ran simulations of solute transport in 3D fracture network systems to capture and track the evolution of the mixing front interface through time.

Angel Hernandez

Program: Undergraduate Student
School: University of Colorado Boulder

Group: CCS-2
Mentor: Nicole Lloyd-Ronning
Discipline: Earth and Space Sciences
Subject Area: Astrophysics
LA-UR-23-27640

XTREME PROGENITORS OF GAMMA-RAY BURSTS

Gamma-ray bursts (GRBs) are the most luminous explosions in the universe. Observations have confirmed that not all GRBs are the same, and their progenitors still remain a mystery. During this presentation, we'll discuss a specific progenitor which involves a massive star and a closely orbiting compact object. With this binary system, we examine how the tidally locked compact object influences the angular momentum of the massive star for a variety of initial conditions using the numerical tool-Modules for Experiments in Stellar Astrophysics (MESA) to accomplish this. The high-performance computing (HPC) Chicoma is used to run these various simulations along with conducting data analysis. We seen that the companion does indeed have an effect on the massive star's angular momentum and present the groundwork for upcoming work regarding the system's atmosphere.

Matthew Holmes

Program: Post-Master's Student
School: University of California, Santa Cruz

Group: XCP-8
Mentor: Wendy Caldwell
Discipline: Earth and Space Sciences
Subject Area: Numerical Modeling
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.

Daniel Jensen

Program: Graduate Student
School: New Mexico Institute of Mining and Technology

Group: ISR-2
Mentor: Xuan-Min Shao
Discipline: Earth and Space Sciences
Subject Area: Atmospheric Electricity
LA-UR-23-27985

INSIGHTS INTO LIGHTNING K-LEADER INITIATION AND DEVELOPMENT FROM THREE DIMENSIONAL BROADBAND INTERFEROMETRIC OBSERVATIONS

A K-leader is a discharge process that occurs at the later stage of a lightning flash. It retraces the path established by earlier discharges and propagates at a high speed of 10—6-107 m/s. Recently we developed a new system called BIMAP-3D that can map lightning radio sources in 3D with high resolution in time and space. We found that K-leaders commonly speed up initially from 106 to 107 m/s and then gradually slow down to a stop. Other branches in the lightning flash are found to affect the K-leader speed as it approaches and passes the branch junctions. After the occurrence of a K-leader radio emissions are shut off for a few milliseconds. After that, scattered radio sources reappear in an expanding region, both extending the branch and expanding back towards the starting point of the lightning. These apparent twinkling radio sources lead to the start of the next K-leader.

Daniel Kozar

Program: Graduate Student
School: University of California, Davis

Group: EES
Mentor: Yu Zhang
Discipline: Earth and Space Sciences
Subject Area: Ecology
LA-UR-23-28256

SPATIAL SIGNATURES OF BIOLOGICAL SOIL CRUSTS AND COMMUNITY LEVEL SELF-ORGANIZATION IN DRYLANDS

Biological soil crusts (BSCs) play a significant role in regulating ecohydrological dynamics in drylands and the redistribution of scarce water in space. While the role of BSCs is largely tied to the abundance and spatial configuration of their patches, little has been done to understand their patches and what drives variation in their patch attributes. To characterize the spatial signatures of BSCs, we analyzed the principal components (PCs) of BSC patches, their interactions with vascular plants, and their drivers from Bayesian regression using ultra-high-resolution classifications of unmanned aerial vehicle (UAV) imagery at 26 sites in the Southwest United States. We find that light cyanobacteria BSCs likely have the capacity to respond to environmental stress through adjusting patch shape while more sensitive dark-mixed BSCs cannot. Cyanobacteria BSCs also likely ameliorate stress through promoting runoff to nearby sink patches. Our findings suggest that self-organization in drylands likely occurs at the community level.

Richard Larson

Program: Graduate Student
School: University of Texas at Austin

Group: EES-16
Mentor: Mohamed Mehana
Discipline: Earth and Space Sciences
Subject Area: Energy Resource Engineering
LA-UR-23-27837

REDISTRIBUTION OF RESIDUAL CO2 DUE TO INTERFACIAL PRESSURE DRIVEN MASS TRANSPORT IN HETEROGENEOUS PORE STRUCTURES

A key benefit of geologic sequestration of carbon dioxide is the capability of long duration, stable, and safe sequestration. As such, the engineered and exploited natural trapping mechanisms of a CO2 injection project are used to optimize and design secure storage projects. Structural, residual, dissolution, and mineral trapping are all known trapping mechanisms which may be favored in various geologic settings. Herein, it is suggested that interactions of some of these trapping mechanisms in certain settings may show additional security in already utilized methods. When these capillary barriers are breached, particularly in the caprock scenario, containment within the desired injection zone may be at risk, leading to slowed or halted operations, and leakage risk. Fine grain zones in the bedforms generally create higher capillary pressures and trap smaller CO2 bubbles, or globules, with higher interfacial curvature, leading to nonuniform dissolution and equilibrium states. A phenomenon called Ostwald Ripening, which is controlled by the diffusive mass transfer, may facilitate the transfer of dissolved CO2 from finer grained regions to their adjacent course-grained regions, disturbing the equilibrium of the residual CO2 bubbles. In this study, the lattice Boltzmann method (LBM) is used to conduct pore-scale simulations of integrated two-phase flow and species mass transport. Quantification of the transient dissolution rate of CO2 in brine, the temporal evolution of bubbles' rearrangement due Ostwald Ripening, and the possibility of mass (e.g., CO2 bubbles) exchange between the fine and coarse-grained layers are conducted.

Yerkezhan Madenova

Program: Post-Master's Student
School: Nazarbayev University

Group: EES-16
Mentor: Luke Philip Frash
Discipline: Earth and Space Sciences
Subject Area: Geomechanics

LA-UR-23-27934

QUAKES WITHOUT SHAKES

Induced seismicity and poor fluid circulation are limiting the use of the Enhanced Geothermal Energy (EGS) for clean electrical power generation. To confront this problem, we propose fracture caging where boundary production wells are drilled around an injection zone to contain fluid and limit seismic risk. Prior work has shown that tensile fractures can be caged, but tensile fractures do not cause seismicity. Our project investigates fracture caging in shear faults because such faults are the primary drivers for seismicity during EGS stimulation. We inject fluid into a critically stressed shear fault and attempt to cage this fluid to limit seismic magnitudes. Our variables include injection rate, fluid induced versus mechanically induced shear, and the size of the fracture cage. Meanwhile we measure acoustic emissions, flow rates, and pressures. Our results prove that boundary wells can cage shear in faults which is a major success for advancing geothermal energy technologies.

Sarah Maebius

Program: Post-Master's Student
School: Imperial College London

Group: EES-14
Mentor: Jon Schwenk
Discipline: Earth and Space Sciences
Subject Area: Environmental Data Science
LA-UR-23-27760

INVESTIGATING HUMAN IMPACTS ON STREAMFLOW IN THE COLORADO RIVER BASIN

Around 40 million people rely on the Colorado River Basin (CRB) as a water source, but reservoir storage has been declining over the past 5 years. Accurate streamflow predictions are necessary to prevent downstream flooding, and ensure water availability for consumption, power, and drought storage. Regional Long Short-Term Memory (LSTM) models struggle to predict next-day streamflow for basins with human impacts, such as reservoir operations, and need additional data inputs to improve accuracy. Our study identifies basins influenced by upstream reservoirs by training an LSTM on pre-dam streamflow and predicting on post-dam streamflow for 96 sites across the CRB. Regions where the LSTM performed well on pre-dam data but poorly on post-dam data were considered human-impacted. A separate post-dam LSTM was trained with additional data sources such as irrigation consumption to increase prediction accuracy. Our LSTM improved streamflow predictions on basins with a high level of human influence.

Agnese Marcato

Program: Graduate Student
School: Politecnico di Torino

Group: EES-16
Mentor: Javier E. Santos
Discipline: Earth and Space Sciences
Subject Area: Computational Earth Science
LA-UR-23-27417

JOURNEY OVER DESTINATION: DIFFERENTIABLE SENSOR PLACEMENT ENHANCES GENERALIZATION

Recreating complex fields from limited data points is challenging across various scientific domains. This challenge is crucial in tasks such as recovering spatio-temporal fields using sensor data. Given the prohibitive costs of specialized sensors and the inaccessibility of regions of the domain, achieving full field coverage is typically not feasible. Therefore, the development of algorithms that improve sensor placement, which make the most of a predefined learning algorithm, is of significant value. In this study, we introduce a general approach that employs differentiable programming to enhance sensor placement, thereby improving field reconstruction. Our approach enables the training of sensor locations using an end-to-end differentiable process. We evaluated our method using two distinct datasets; the results show that our approach yields better sensor positions compared to random placements enhancing learning. Our method has the potential to increase data collection efficiency, enable more thorough area coverage, and reduce redundancy in sensor deployment.

Micalah Miller

Program: Post-Bachelor's Student
School: St. John's College

Group: ISR-1
Mentor: David Gerts
Discipline: Earth and Space Sciences
Subject Area: Space Science and Nuclear Physics
LA-UR-23-27583

DEVELOPMENT OF ANISOTROPIC INDEPENDENT RAYS USING GEOMETRY-ONLY METHODS

Correct calculations of gamma-ray transport through the atmosphere is important for the understanding of space-based measurements. However, current methods to achieve this are computationally expensive. The objective of this project is to create transport matrices that will aid in the understanding of impulsive gamma ray emissions for each emission energy, source direction, and source altitude. This works presents preliminary steps for the creation of the matrix which includes cross sectional values, ray attenuation in one layer of atmosphere, and ray attenuation through the entire atmosphere. By the end of this project, we expect to have the full scattering matrices and a benchmark comparison to Monte Carlo N-Particle Transport Code (MCNP). This method will provide a significant calculation time improvement over MCNP using standard variance reductions techniques, as much as 104 times faster.

Shifat Monami

Program: Graduate Student
School: Auburn University

Group: EES-16
Mentor: Nathan Conroy
Discipline: Earth and Space Sciences
Subject Area: Geoscience
LA-UR-23-27666

URANIUM SPECIATION, SORPTION, AND TRANSPORT AT AN IN SITU RECOVERY MINE: INSIGHTS FROM GEOCHEMICAL MODELING

Uranium in situ recovery (ISR) mining involves the leaching of uranium from roll-front deposits by oxidative dissolution using carbonate rich oxygenated solution, known as a lixiviant. The leachates are pumped to the surface for uranium recovery using ion exchange resins. After ISR operations are complete, the subsurface environments undergo restoration to reduce the concentration of uranium and other constituents in the groundwater. The restoration is usually accomplished by sweeping the mined site with formation water followed by several sweeps with reverse osmosis water. Other restoration approaches include introducing reducing agents such as sodium dithionate to reduce U(VI) to the significantly less soluble U(IV), or by introducing complexing agents (e.g., phosphates) to precipitate U(VI) phases. The efficiency of site restoration depends on the local hydro and geochemical conditions, which determine uranium sorption/precipitation and transport. Laboratory column studies are commonly employed to optimize the leaching and restoration operations. However, these tests are very time consuming and require expensive core material, making it impractical to experimentally test every possible groundwater restoration strategy. Fortunately, uranium speciation has been extensively studied and there is rich thermodynamic data set, which can be coupled with geochemical modeling to predict experimental outcomes and prioritize the column experiments that should be performed in the laboratory. In this study, geochemical modeling software PHREEQC was used to conduct initial evaluations of the column effluent, assessing the potential for adsorption, reduction, and/or mineral precipitation. PHREEQC is implemented in a 1D transport model to simulate the geochemical reactions occurring within the column. The initial parameters utilized in the model are derived from field and laboratory data collected from the Church Rock uranium mining site within the historic Grants Mining District in McKinley County, New Mexico. The results of this study aim to enhance our understanding of the mechanisms involved and the effectiveness of immobilizing uranium under various geochemical conditions. By shedding light on these aspects, this research contributes to the overall knowledge base of groundwater restoration strategies following uranium ISR mining.

Anika Nath

Program: Undergraduate Student
School: Massachusetts Institute of Technology

Group: ISR-6
Mentor: Nina Lanza

Discipline: Earth and Space Sciences
Subject Area: Planetary Science
LA-UR-23-27772

EXAMINING ROCK COATINGS WITH LIBS SPECTRAL AND ACOUSTIC DATA

Laser-induced breakdown spectroscopy (LIBS) is an analytical technique used by SuperCam on Mars to analyze the chemical composition of rocks. The laser heats the rock, transforming it into plasma, which generates a shockwave detectable by the SuperCam microphone. By ablating the sample, LIBS allows for investigating chemical stratification with depth. However, the LIBS spectra data is somewhat ineffective in detecting composition transitions between similar coatings and host bedrocks. The LIBS acoustic provides additional information on rock properties, such as hardness. In this study, we compared the laboratory data of two rocks, one with a coating and the other uncoated, using both LIBS acoustic and chemical analysis. The results indicate that acoustics can identify the transition between the coating and the rock, offering a potential solution to overcome LIBS' limitations in discerning such transitions.

Siobhan Niklasson

Program: Graduate Student
School: New Mexico Tech

Group: EES-17
Mentor: Charlotte Rowe
Discipline: Earth and Space Sciences
Subject Area: Geophysics
LA-UR-23-20089

COMPARISON OF AMBIENT NOISE BETWEEN OCEAN-BOTTOM SEISMIC NETWORKS

Seismic sensors have traditionally been largely restricted to on-land installations, yet the oceans cover roughly 70% of the Earth's surface. The ambient noise level recorded by ocean-bottom seismometers (OBS) is generally much higher than ambient noise levels on land, and details of the seafloor noise regime are not well described. We present progress in evaluation of OBS noise characteristics at temporary network deployments distributed throughout the Earth's oceans. We choose a single type of instrument in order to focus our analysis on noise variations due to oceanographic and geologic factors. Our long-term objective is to characterize source and path effects of seafloor noise across the globe by combining existing noise observations with predictions of noise from known sources, and to use this characterization to guide site selection and optimization of seafloor seismic array geometry.

John Ortiz

Program: Graduate Student
School: Johns Hopkins University

Group: EES-16
Mentor: Phil Stauffer
Discipline: Earth and Space Sciences
Subject Area: Planetary Science
LA-UR-23-28109

SUB-DIURNAL METHANE VARIATIONS ON MARS DRIVEN BY BAROMETRIC PUMPING AND PLANETARY BOUNDARY LAYER EVOLUTION

In recent years, the Sample Analysis at Mars (SAM) instrument on board the Mars Science Laboratory (MSL) Curiosity rover has detected methane variations in the atmosphere at Gale crater. Methane concentrations appear to fluctuate seasonally as well as sub-diurnally, which is difficult to reconcile with an as-yet-unknown transport mechanism delivering the gas from underground to the atmosphere. We consider barometrically-induced transport of methane from an underground source to the surface, modulated by temperature-dependent adsorption as a mechanism to potentially explain the fluctuations. The subsurface fractured-rock seepage model is coupled to a simplified atmospheric mixing model to provide insights on the pattern of atmospheric methane concentrations in response to transient surface methane emissions, as well as to predict sub-diurnal variation in methane abundance for the Northern Summer period, for which we propose two strategic SAM-TLS samples during Curiosity's potentially final sampling campaign.

Dulcie Quinn

Program: Undergraduate Student
School: University of Arizona

Group: T-5
Mentor: Pedro Resendiz
Discipline: Earth and Space Sciences
Subject Area: Plasma Physics
LA-UR-23-27384

INTERPRETATION OF MAGNETOSPHERIC COLD PARTICLE DISTRIBUTION FUNCTIONS MEASURED WITH ACTIVE SPACECRAFT CONTROL

The cold (~eV) particle populations within the Earth's magnetosphere play an important role in the dynamics of the magnetosphere. However, relatively few studies have focused on the cold electron and cold ion populations of the magnetosphere due to difficulties associated with obtaining measurements. A promising technique to measure the full distribution of cold particle populations is through active spacecraft control. In this project, our goal is to interpret particle fluxes under the effect of active spacecraft control in terms of the parameters of the background plasma (density and temperature), numerically computing from particle fluxes obtained by kinetic simulations and lab experiments.

Lucas Tiede

Program: Undergraduate Student
School: New Mexico State University

Group: EES-14
Mentor: Zachary Robbins
Discipline: Earth and Space Sciences
Subject Area: Earth Systems Modeling
LA-UR-23-27250

SIMULATING FUTURE RISK OF PLANT HYDRAULIC FAILURE AT MANAUS, BRAZIL USING A DYNAMIC VEGETATION MODEL

Accuracy in climate modeling is crucial in order to appropriately address our world's climate emergency, to understand future change, and to mitigate ecological and societal damage. To accomplish this, we are parameterizing an Energy Exascale Earth System Model – Functionality Assembled Terrestrial Ecosystem Simulator (E3SM-FATES) with a plant hydrodynamics (HYDRO) model linking climate, vegetation, hydrological and soils data for a site in Manaus, Brazil. There is a risk in these forests that future warming and drought could increase the risk of mortality caused by hydraulic failure. We will be parameterizing the model using LANLs High Performance computing (HPC) resources to simulate various plant traits and understand their response to local droughts under the current and future climate conditions We then will use this model to understand the risk of plant hydraulic failure and its effect on the water and carbon cycles.

Engineering

Andrew Ahn

Program: Graduate Student
School: University of Oregon

Group: MST-7
Mentor: Rachel Collino
Discipline: Engineering
Subject Area: Materials Science/Testing
LA-UR-23-27831

DIGITAL IMAGE CORRELATION FOR CHARACTERIZATION OF ADVANCED POLYMER AND COMPOSITE MATERIALS

Digital image correlation (DIC), applied in tandem with classical mechanical testing of soft materials, can provide full-field information regarding local deformations. This approach is especially motivated for polymers and composite components created via traditional or additive manufacturing techniques that induce local polymer chain alignments and/or printed structures that induce non-uniform strain gradients under applied stress. However, this capability also introduces practical testing challenges – this poster will discuss the application of DIC to a variety of soft materials, as part of several efforts in MST-7 targeting novel materials and processes with tailored mechanical respon

Elijah Boland

Program: Graduate Student
School: Missouri University of Science and Technology

Group: W-13
Mentor: Edward Lum
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-27855

ENERGETIC GODIVA-IV RADIATION EXPERIMENT TESTBED

The purpose of the proposed experiment is to study and document any measurable change in the temperature and displacement of a HEU sample during a Godiva-IV pulse. The experiment consists of four independent experiment packages. Three experiment packages shall contain one HEU sample while the fourth experiment package shall contain an Aluminum sample with a flexible membrane to obtain background data for the PDV probes. The background experiment package shall be pulsed at maximum Godiva-IV power (which correlates to a fuel temperature rise of 250 degrees) on the first day of the experiment while the three other packages shall be pulsed at maximum Godiva-IV over the next three days with one package being pulsed per day. This experiment shall serve as a scoping investigation for potential future SNM tests. The experiment objective is to expose a HEU sample to a Godiva-IV pulse and obtain sample time-dependent temperature and displacement values.

Kristin Boyler

Program: Undergraduate Student
School: University of Iowa

Group: T-3
Mentor: Milovan Zecevic
Discipline: Engineering
Subject Area: Mechanical Engineering

LA-UR-23-27456

MODELING HIGH-RATE DEFORMATION OF PBX

High-rate deformation of a composite consisting of energetic crystal particles and polymer binder (PBX) is studied with a finite element software. The composite impacts a rigid wall causing the kinetic energy to convert into thermal and potential energy. The increase of thermal energy is caused by rising temperature due to dissipation and thermo-elastic coupling. Within the energetic crystals, there are small volumes of high temperature, i.e., hot spots. Hot spots are important for predicting if the energetic crystals will react. Resolving hot spots in simulations requires sub-micron element size which is accompanied by significant computational costs. To minimize computational costs, two methods are explored: using a submodel and Adaptive Mesh Refinement (AMR). In the submodel approach, impact simulations are run with a coarse mesh. Small volume from impact simulations is refined and rerun with boundary conditions driven by the full model. AMR allows for local refinement of elements during the course of simulation based on a chosen criterion.

Nathanael Breed

Program: Undergraduate Student
School: Liberty University

Vanessa Kalenits

Program: Undergraduate Student
School: University of Nevada, Reno

Group: J-NV
Mentor: Steven Pemberton
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27350

DIAGNOSTIC TEST BED FOR HIGH EXPLOSIVE EXPERIMENTS

One of the primary goals of J-NV is the high-fidelity diagnosis of high explosives experiments. Diagnostics range from high-speed cameras to visually capture what is happening to flash x-ray equipment to snapshot fragment velocities. Due to the complexity of these diagnostics, extensive training is required for personnel to gain adequate knowledge and experience to successfully operate the equipment and interpret the results. To help expedite this training process, a diagnostic test bed was developed to simulate, on a micro-scale, the visible, audible, and kinetic elements of a full scale HE experiment in order to accommodate the testing of a diverse set of diagnostics. This project required both electrical and mechanical engineering skill sets. The benefits posed by this project are substantial, as it will save both time and money for the group and enable the development of new, advanced diagnostic and instrumentation technologies.

Galen Brown

Program: Post-Master's Student
School: Worcester Polytechnic Institute

Group: E-6
Mentor: Shannon Scott
Discipline: Engineering
Subject Area: Non-Destructive Testing

LA-UR-23-27401

PARAMETER ESTIMATION EVALUATION FOR X-RAY TOMOGRAPHY CALIBRATION

In order to produce high quality reconstructions, X-ray Computed Tomography (X-CT) systems must first be calibrated by scanning an object with known geometry (a phantom). After the phantom has been scanned, the X-CT system's parameters can be computed. There are several competing methods in the literature for performing this computation, each of which produces slightly different results. In this work, I first construct a metric by which different reconstructions can be directly compared to one another without knowing the underlying ground truth of the system parameters. I then present a sequential optimization method to improve initial parameter estimation, and demonstrate its performance on simulated and real X-CT calibration series.

Sergio Bugosen

Program: Graduate Student
School: Carnegie Mellon University

Group: A-1
Mentor: Robert Parker
Discipline: Engineering
Subject Area: Chemical Engineering
LA-UR-23-27516

A COMPARISON OF CONVERGENCE RELIABILITY FOR FLOWSHEET OPTIMIZATION WITH SURROGATE AND FIRST-PRINCIPLES UNIT MODELS

The United States has set ambitious goals for the future, aiming to reduce greenhouse emissions by 50-52% below 2005 levels by 2030. Additionally, it is looking to reach 100% carbon pollution-free electricity by 2035. To meet these objectives, chemical processes that manufacture hydrogen from waste or natural gas must be modeled to optimality to satisfy product specifications, as well as safety, economic, and environmental constraints. However, classical optimization of a chemical process is challenging due to the number of variables and algebraic equations defining each unit operation, as well as the nonlinear complexity of these first principles models. Convergence of these optimization models is sensitive to initial guess, scaling, and problem formulation. To improve solver convergence reliability when optimizing a chemical process flowsheet, we implement data-driven optimization based on surrogate modeling.

Olivia Cantrell

Program: Undergraduate Student
School: New Mexico Institute of Mining and Technology

Group: ISR-1
Mentor: Ernst Esch
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-28088

ADRESS INTERLOCKING MINI-PALLET "BEETLE" DESIGN

The Automated Drum Retrieval and Storage System (ADReSS) Project aspires to fully automate the drum storage and retrieval process that is ongoing at the Transuranic Waste Facility (TWF). By fully automating the drum storage and retrieval process, the risk of accidental spill, drum damage, and contamination is lowered significantly. In this automating endeavor, two “mini-pallet” prototypes were designed to allow for seamless drive within the shelving system. These new designs allow for one drum per pallet for simpler drum transportation as well as drum locks for stability. The main feature on the new prototypes is the interlocking system which allows the pallets to slide together in order to prevent wedging on the shelving system. The ADReSS Project aims to benefit the LANL mission by ultimately optimizing one of the Laboratory’s most vital tasks of waste management.

Miguel Chacon Cuesta

Program: Undergraduate Student
School: Arizona State University

Group: P-4
Mentor: Vincent Garcia
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27423

FEA OF PHELIX LOWER COMPRESSION RING

PHELIX is a portable, pulsed-power capacitor bank driver of hydrodynamic experiments at LANSCE's Proton Radiography station. The experimental load, the cassette, is new for each shot, but the rest of the system is designed for reliable, predictable performance with minor maintenance. Acting as a high-current crush joint between the transformer and cassette, PHELIX has a lower compression ring. Currently, the cassette extraction process is inefficient due to gulling between the ring and liner. The objective is to conduct an FEA to simulate the mechanical load applied onto rings of different materials. This will determine materials that meet the deformation specifications without experiencing gulling allowing for a smoother cassette removal. The project includes calculating the external load the bolts apply onto the ring and developing an FEA simulation that accurately depicts the ring's displacement for a given material; in this case, Aluminum 1060-O and OFHC Soft Copper.

Carlos Chacon Cuesta

Program: Undergraduate Student
School: Arizona State University Polytechnic Campus

Group: PT-5
Mentor: Chris Wetteland
Discipline: Engineering
Subject Area: Robotics Engineering
LA-UR-23-27248

METHODOLOGIES FOR ATMOSPHERIC MOISTURE REMOVAL IN PRODUCTION ENVIRONMENTS

The purpose of the Vacuum Moisture Analysis project is to conduct a series of experiments that will analyze and help understand how water molecules behave in a vacuum environment similar to those commonly found in the chambers and glove boxes used to handle plutonium at Los Alamos National Laboratory (LANL). . The end goal of the project is to identify a set of methods and techniques that can effectively and efficiently improve the removal of moisture in production environments. The areas of primary interest are the effects on the chamber's pump down time to a set pressure after: exposing the vacuum to the surrounding environment for variable time intervals and at differing humidity levels, undergoing different surface pre-treatments, and the application of different water removal techniques.

Jonah Chad

Program: Graduate Student
School: University of Michigan

Group: C-CDE
Mentor: Kwan-Soo Lee
Discipline: Engineering
Subject Area: Additive Manufacturing
LA-UR-23-26733

QUALIFICATION OF ADDITIVELY MANUFACTURED CERAMICS

Additive manufacturing (AM) has become a desired manufacturing alternative, due to its capability to fabricate complex geometries at high resolution, ability to decrease cost/time, and reduced assembly when compared to traditional manufacturing methods. However, AM parts lack consistency, in part due to limited qualification of materials and processes. This is especially true of ceramics, where applications are limited due to material properties as well as a lack of understanding how process constraints impact part performance. This project seeks to advance the understanding of process-structure-property-performance relations for ceramic AM through the development of models that are validated by experimentation. This research will improve understanding of ceramic AM by increasing the range of properties that are attainable by AM, producing functional parts that are unable to be fabricated using traditional manufacturing methods, and creating printed parts that are both accurate and consistent.

Emily Chavez

Program: Undergraduate Student
School: New Mexico Institute of Mining and Technology

Group: Q-18
Mentor: Mike Seinzig
Discipline: Engineering
Subject Area: Mechanical Engineering

LA-UR-23-28209

PYTHON CODE DEVELOPMENT FOR ANALYZATION OF WATER ABSORPTION IN ESTANE® 5703 POLYMERS

Estane® 5703 (E03) is commonly used as a binder in plastic bonded explosives (PBXs), such as PBX 9501. The stability of E03 determines the stability of PBX 9501. E03 is prone to hydrolysis, resulting in decreased molecular weight and poor mechanical properties. Hence, it is essential to assess risks relevant to E03 lifetime aging when gaining and losing moisture content. MST-7 scientists used Dynamic Vapor Sorption (DVS) instrumentation to study the absorption and desorption of E03 when it is exposed to various temperature and humidity conditions. Large amounts of data have been collected. To improve the efficiency of the data analyzation, several iterations of Python code were developed to process the data. These include reprocessing raw data, fitting the data using the mass transport equation, and calculating the diffusion coefficient and water absorption capacity under various conditions. The Arrhenius laws of water diffusion in E03 were obtained.

Srinidhi Chillara

Program: Graduate Student
School: University of New Mexico

Group: MPA-11
Mentor: John Greenhall
Discipline: Engineering
Subject Area: Machine Learning
LA-UR-23-27488

NONINVASIVE ACOUSTIC RESONANCE SPECTROSCOPY TO MEASURE PRESSURE IN SEALED CANS USING MACHINE LEARNING

The idea of using Noninvasive Acoustic Resonance Spectroscopy (ARS) for measuring pressure in the cans is critical in wide range of applications where the direct measurement of the internal pressure is not possible. The examples include disposal of used hazardous gas containers and underwater/space salvage and rescue operations of the systems where the pressure gauges may be broken or unreliable. ARS provides noninvasive measurements of the cans or of any sealed systems by vibrating the exterior of the system and measuring the acoustic spectrum of the entire system, which is highly sensitive to the system geometry, materials and the environment. Many techniques have been proposed in the literature for specific applications. However, extracting useful and meaningful information from the noisy ARS measurements is still an open challenge. The proposed study aims at trying to implement different machine learning models such as convolutional neural networks and recurrent neural networks based on long short-term memory networks to see if these models can estimate the internal pressure of the cans from the ARS data. We train and test each model to estimate the pressure from experimental ARS measurements in commercially available vacuum cans. This enables comparing each model and analyzing the effect of the ARS frequency window used.

John Corder

Program: Graduate Student
School: Texas A&M University

Group: NEN-1
Mentor: Sarah Sarnoski
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-27895

DYNAMIC BACKGROUND ANALYSIS FOR NUCLEAR MATERIAL ACCOUNTING

Quantifying nuclear material using nondestructive assay measurement systems requires subtraction of background for accurate analysis, as high backgrounds can contribute to uncertainty. The movement of nuclear material creates a dynamic background that can contribute to inaccurate measurements on a detector. This work aims to simulate different dynamic neutron-background environments and how background affects measurements on a thermal neutron counter (TNC). The methodology to this work is modeling a TNC with neutron-emitting sources outside of the detector at various positions. The simulations are run in MCNP to analyze the variation in detector response as a function of background source location. This analysis provides insight on reducing background effects and improving background subtraction for material accounting.

Allison Davis

Program: Post-Master's Student
School: University of Wyoming

Group: E-1
Mentor: David Mascarenas
Discipline: Engineering
Subject Area: Computer Vision
LA-UR-23-27411

QUANTIFYING IMAGE RECONSTRUCTION BY NEURAL RADIANCE FIELDS USING SPATIAL FREQUENCY ANALYSIS

A neural radiance field (NeRF) is a multilayer perceptron model that can be trained on a sparse set of images taken at different viewing angles to create a 3D volumetric model of the scene, and generate arbitrary novel views. Image reconstruction by a NeRF is often judged in a qualitative manner by visually comparing the ground truth images to reconstructed images. This work seeks to verify the accuracy of reconstructed images quantitatively by comparing the spatial frequency content of ground truth images to that of the reconstructed images. These comparisons are performed at different iterations during the learning process to better understand how the spatial frequency content is learned during training time. By understanding how the spatial frequency content evolves in the NeRF model, we develop a better understanding of the accuracy of the image reconstruction that is achieved by NeRF.

Nadezda Draganic

Program: Undergraduate Student
School: University of California, Davis

Group: AOT-MDE
Mentor: Bhavini Singh
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-26861

FLOW INDUCED VIBRATION EFFECTS ON MO-100 DISCS

We explore the effect of disc vibration on mass loss in Mo-100 discs (25.4 mm diameter, 0.737 mm thick. A stack of Mo-100 discs is placed under high pressure helium gas (approximately 260 psi to 315 psi) and run in a closed loop system whose flow is driven by an industrial blower. The flow rate is varied from 0 to 75 g/s, with the highest flow rate corresponding to a Reynolds number of 14000. Disc motion is measured using multiple techniques, with this work focusing on microphone measurements to estimate disc vibration frequency. The measurements are analyzed using signal processing techniques in MATLAB. The mass is measured before and after each experiment and then compared to the microphone measurements. SolidWorks is used to design the experimental components like soundproof boxing around the microphone. Additional studies include the design of a small wind tunnel and fluid dynamic simulations in Ansys.

Micky Dzur

Program: Undergraduate Student
School: Texas A&M University

Group: XCP-3
Mentor: Jerawan Armstrong
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-27779

OKTAVIAN MODELING AND ANALYSIS WITH MCNP6.3

The goal of this project is using the Monte Carlo N-Particle (MCNP)1 transport code to verify the application of variance reduction techniques on the unstructured mesh (UM) geometry feature. The traditional MCNP geometry feature, known as constructive solid geometry (CSG), creates models by combining surfaces to create volumes denoted as cells. We used the MCNP5 CSG input file released with the Oktavian pulsed sphere benchmark experiment in the Shielding Integral Benchmark Archive and Database (SINBAD) for this verification. We modified the CSG input files of the Oktavian experiments for use with MCNP6.3 and compared the calculation results for the old and new CSG input files. The MCNP UM feature requires a solid 3D model to be decomposed into finite elements using an external software. CUBIT, developed by Sandia National Laboratories, was used to create and mesh the Oktavian models for this work. We performed both UM and CSG calculations using various variance reduction techniques to compare and verify the UM results against the CSG results.

Marina Espinosa

Program: Undergraduate Student
School: New Mexico State University

Group: W-13
Mentor: Gretchen Ellis
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27314

PREDICTION CAPABILITIES OF ABAQUS MODELING FOR A PRELOADED BOLTED JOINT COMPARED TO EXPERIMENTAL RESULTS

A bolted joint is one of the most common mechanical design methods for connecting structural components and is considered a critical part of any assembly. Engineers often underestimate the complexity of bolted joints, which can lead to ineffective designs and inaccurate model simulations of joint stiffness and bolt failure. To assess the true behavior of preloaded joints we compared the predictions of calculated closed-form solutions and Finite Element Analysis (FEA) models to various experimental data. Engineers regularly use closed-form solutions, empirical data, and model simulations to optimize bolted joint designs and assess structural integrity while estimating failure modes. However, the accuracy of these predictions relies heavily on input parameters. Therefore, experimental validation is crucial to ensure the reliability of closed-form solutions and FEA models. The results of our work provide important guidance for design engineers and engineering analysts on modeling and analyzing bolted joints, and the inherent uncertainties therein.

Dylan Frank

Program: Undergraduate Student
School: Texas A&M University

Group: NEN-1
Mentor: Lauren Janney
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-27768

SIMULATING AN HPGE DETECTOR TO ACCELERATE NUCLEAR OPERATIONS

Frequent nuclear material inventories and long operational pauses for inventory reconciliations in complex nuclear production facilities can significantly reduce operational efficiency. To improve nuclear material control and reduce the impact of required inventories, a diverse toolkit of detectors may be deployed within a facility to dynamically track and account for in-process nuclear material. One set of tools under development include validated computer models of high purity germanium gamma spectroscopy detectors using the Monte Carlo N-Particle® (MCNP®) radiation transport code. These models are validated through the analysis of carefully planned laboratory experiments. This project focuses specifically on the Detective® X, a portable gamma detector designed by ORTEC®. Additionally, a Python package called speTools has been developed to facilitate the validation of radiation transport models of high-fidelity gamma detectors by reproducing the measured detector characteristics of efficiency, resolution, and spatial sensitivity.

Ryan Garcia

Program: Undergraduate Student
School: Texas Tech University

Group: W-10
Mentor: Francis Martinez
Discipline: Engineering
Subject Area: Civil Engineering
LA-UR-23-27897

USING POLYCARBONATE SHIELDING FOR EXPLOSIVE SAFETY

The prevention and mitigation of potential hazardous fragments is an important aspect of weapons safety and response. The goal of this project is to help identify material(s) that may be used for mitigating fragments in the case of incidental detonation of co-located high explosives (HE) assemblies. Polycarbonate (PC) is an amorphous thermoplastic which is transparent in nature and possesses the material properties of having a low coefficient of thermal expansion alongside high impact, tensile, shear and flexure strength. PC shielding has demonstrated its strength through ballistic, pressure, and explosive testing which makes it a material of interest for its potential to protect against a sympathetic detonation of co-located HE devices housed within the same multi-project facility. By researching the potential uses of PC, work can be conducted that may allow for PC shielding to be implemented into existing Department of Energy explosives safety and weapons response guidelines and standards.

Nicholas Garcia

Program: Undergraduate Student
School: Texas A&M University

Group: PT-02
Mentor: Wendel Brown

Discipline: Engineering
Subject Area: Control Systems Engineering
LA-UR-23-27412

HIGH PRECISION MEASUREMENT WITH OPTICAL MICROMETER

Taking proper measurements when machining a part can plays a crucial role in determining whether the features of a micro tensile sample meet dimensional requirements. If a micro tensile sample is out of tolerance, it may have to be reworked in order to get it into tolerance, or even completely discarded. However, it is possible that, if measured incorrectly, a micro tensile sample could be in tolerance and appear outside of this range. By measuring with a precision optical micrometer and filtering the data, it is possible to see if a micro tensile sample is within specification on the lathe. Additionally, certain additions can be made in order to automate this process and make it more efficient overall. The whole process plays a key role in the machining, measurement, and testing of various parts used at the laboratory. This poster describes the methodology used to fully characterize a large dataset generated by the optical micrometer. I used a combination of C++ and Python algorithms to condense the data before modeling. Graphing capabilities found within Python allow for easy interpretation of the dataset by the machinists.

Bradley Gladden

Program: Graduate Student
School: University of Texas at Austin

Group: XCP-3
Mentor: Jerawan Armstrong
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-27773

MCNP6.3 VERIFICATION OF CSG AND UM ATHENA-I MODEL

This poster presents the modeling and simulation in Monte Carlo N-Particle (MCNP) transport code for an energy tuning assembly known as Athena-I. The Athena-I experiment was conducted at the National Ignition Facility (NIF) by the Air Force Institute of Technology (AFIT) where MCNP6.1 was used to create a constructive solid geometry (CSG) input for experimental analysis. Our goal for this project is to develop unstructured mesh (UM) models of Athena-I and verify MCNP6.3 UM results with MCNP6.3 CSG results. Based on the Athena-I CSG input file, we use CUBIT, a mesh generation software package developed by Sandia National Laboratory, to create two UM models. We generate CUBIT journal files for a hexahedral and tetrahedral UM model. The UM models exported from CUBIT are then pre-processed and used for MCNP UM simulations. Variance-reduction techniques in MCNP were developed to improve computing efficiency. Weight-Windows (WW) is one of MCNP variance reduction techniques. Applying WW to complex systems is not easy, and iterations are typically needed. We use the WWG card to generate the cell-based weight window file. When applying WW to the CSG calculation of Athena-I, the computing time is significantly faster. However, there is no improvement when applying the same WW parameters for UM calculations.

Shayna Gomez

Program: Undergraduate Student
School: Texas Tech University

Group: AOT-RFE
Mentor: Maria Sanchez-Barrueta
Discipline: Engineering
Subject Area: Electrical and Radio Frequency
LA-UR-23-27260

RADIO FREQUENCY POWER DETECTOR UPGRADE FOR LANSCE

The Linear Accelerator Neutron Science Center (LANSCE) uses 50 high-power radio-frequency amplifiers as means to provide power to its accelerating cavities. Each of these amplifier's performance is evaluated based on its forward power and interlocked against excessive reflected power coming back from the cavity in the event of an arc. The device that provides power measurements for the purpose of both measurement and interlocks is the power detector. This device must be calibrated through a detailed procedure and able to store and access an offset indicating the precisely measured coefficient of the power measured in this device (ranging µW – mW) to the real power in the system (10 kW - MW). The original device was installed in the drift tube linac section of LANSCE starting in 2014 and relies on obsolete systems to be recalibrated and programmed. An extensive update to the detector and the calibrating equipment has been performed to continue supporting LANSCE operations for years to come.

Elena Gonzales

Program: Post-Bachelor's Student
School: New Mexico State University

Group: ISR-2
Mentor: Ernst Gonzales
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-28012

ADRESS DRUM LOCK TEST SYSTEM

The Transuranic Waste Facility (TWF) at the Los Alamos National Laboratory (LANL) stores various quantities of transuranic waste created at LANL before it is shipped to the Waste Isolation Pilot Plant (WIPP) for long term storage. The current drum handling procedure at the TWF is labor-intensive, inefficient, and costly. During this process workers are exposed to mechanical and radiation hazards. To combat these risks and optimize the storage system at the TWF the Automated Drum Retrieval and Storage System (ADReSS) was created. Focusing on the characterization and storage of the waste drums, the system will also mitigate any ergonomic issues or hazards present in the waste handling procedure. Automating the characterization and storage process through a robotic system alleviates mechanical hazards and distances workers from the TRU waste, prioritizing ALARA principle. Other benefits include an increase in storage capacity within each warehouse and a reduction in the overall procedure time.

Jalyn Gould

Program: Undergraduate Student
School: New Mexico Institute of Mining and Technology

Group: Q-6
Mentor: Anna Buckthrope
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-28285

FABRICATION OF A MORE ACCESSIBLE FIRING FIXTURE FOR DETONATORS

Detonators need a secure fixture to hold it steady during detonation, so that the diagnostics equipment can accurately record data. Fixtures must be reliable, so that after each print it is a guarantee that it will be the same quality. The front side has two thin lines that the diagnostics equipment uses as a reference point so that it can be positioned to collect data. Buying fixtures often have a long lead time, taking months from ordering to delivery. With more access to 3-D printing, there is a faster and easier way to get our hands on firing fixtures. By translating a previous model into a 3-D design, this allows us to have the ability to print as many fixtures as needed, within hours, on-site. 3-D models allow for more design flexibility and lays the groundwork for customization.

Corinne Jackson

Program: Undergraduate Student
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Group: W-11
Mentor: Nathan Mesick
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27552

BATTERY PACK DESIGN FOR SENSOR NETWORKS: THERMAL ANALYSIS AND SAFETY

Efficient and safe batteries are a critical engineering design consideration for a wide range of technology fields - from large-scale public transportation to nuclear stockpile stewardship. Maximizing power density while protecting from catastrophic failures such as thermal runaway and battery explosion has proven a design challenge for battery packs supplying power to data acquisition systems in harsh environments. In this project, we use thermal simulation to predict peak temperatures for different lithium battery cells in custom battery pack designs. These temperatures are used to assess the thermal safety of each assembly and adjust battery housing design. Housing materials are chosen to mitigate heat concentrations and therefore allow the battery pack a longer life span.

Nancy Joseph

Program: Graduate Student
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Group: CCS-3
Mentor: Kari Sentz
Discipline: Engineering
Subject Area: Electrical Engineering

LA-UR-23-27614

DOMAIN SHIFT FOR POST-DISASTER ASSESSMENT

Computer vision task such as semantic segmentation have a wide range of applications. In the natural disaster domain, segmentation models have been used for damage assessment. In recent years, unmanned aerial vehicles (UAV) have make it possible to identify small objects such as vehicles and pools because the photos are taken closer from the ground. Domain shift occurs when the model is trained in a one domain and tested on another domain. This works explores domain shift using a vision transformer called SegFormer on UAV image datasets: FloodNet and RescueNet. These datasets were created after Hurricane Harvey and Hurricane Michael respectively. These two data sets share common object classes, such as pool, vehicle, water, and tree. Thus model evaluations, such intersection over union (IoU) and pixel accuracy, will be conducted using the SegFormer on the two data set for the common object classes.

Johnathen Kammer

Program: Undergraduate Student
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Elijah Witsenhausen

Program: Undergraduate Student
School: Worcester Polytechnic Institute

Group: E-6
Mentor: Andre Spears
Discipline: Engineering
Subject Area: Computer Engineering

LA-UR-23-27400

X-RAY SAFETY INTERLOCK PLC EMULATOR

E-6 maintains several radiography bays across its various facilities at TA08. Every bay has its own safety interlock implementation with its own limitations and problems. E-6 has set a goal to replace all of the interlock systems with a common adaptable system that may be applied regardless of radiographic bay configuration. In order to test this system safely, there is a need to emulate X-ray system operation to test interlock functionality. We programmed and configured a programmable logic controller (PLC) to simulate a safety system designed for x-ray systems that will be interlocked to avoid accidental use outside of accepted guidelines. PLC uses both buttons on the PLC trainer and human machine interface (HMI) to control the operation of the safety system. For safety shut off for when emergency situations occur the PLC has a relay, safety switches and an emergency shut off button.

Samuel Kilgore

Program: Undergraduate Student
School: Texas A&M University

Michael Rakoski

Program: Undergraduate Student
School: Texas A&M University

Nicholas Kroger

Program: Undergraduate Student
School: Texas A&M University

Sarah Beth Ragan

Program: Undergraduate Student
School: Texas A&M University

Group: M-9
Mentor: William Perry

Discipline: Engineering
Subject Area: Shock Physics
LA-UR-23-27469

SAMURAI EXPERIMENT: SHOCK INITIATED DEFLAGRATION ANALYSIS

With safety being one of the primary missions of the lab, understanding the response of high explosives (HE) to shock loading is paramount. πSURF is a reactive burn model that relates shock sensitivity and microstructure. This model suggests that details of the microstructure, primarily void surface area and deflagration speed (D0), govern the overall reaction rate. Custom PBX 9501 (HMX) with a controlled void size distribution was manufactured allowing the effective void surface area (Ã) to be known. A known void distribution then allows for the isolation of the deflagration speed during shock initiation. We can then observe this phenomena using diagnostics such as Photon Doppler Velocimetry (PDV). We hypothesize that all voids in this formulation will ignite at ~3.5GPa. Because Ã is constrained, quantitative determination of D0 is expected. This directly informs the deflagration component of the πSURF reaction model.

Daniel Kim

Program: High School Student
School: Los Alamos High School

Group: AOT-RFE
Mentor: Sung Il Kwon
Discipline: Engineering
Subject Area: Electrical Engineering
LA-UR-23-27261

FPGA IMPLEMENTATION OF A TUNABLE CAVITY SIMULATOR AND ITS APPLICATION FOR LANSCE ACCELERATOR TESTBENCH

The Los Alamos Neutron Science Center (LANSCE) accelerators feature cavities with different resonance frequencies, Q factors, and beam energies. To stabilize the RF field for beam acceleration, a complex Low-level radio frequency (LLRF) control system is required. Ideally, basic functions and control algorithms of the LLRF system are tested in real-time, but the necessary equipment for testing, such as RF cavities and high-power RF sources, is costly. To address this, we have developed a field-programmable gate array (FPGA) based cavity simulator as a substitute for real cavities. This simulator implements a digital baseband model of a cavity in the FPGA, allowing us to establish an LLRF system testbench where cavity parameters, such as the 3dB bandwidth, can be adjusted to study the signal behaviors of different LANSCE cavities. By comparing the simulation's performance with existing cavities in the LANSCE accelerators, we have successfully verified its effectiveness.

Jessica Lalonde

Program: Graduate Student
School: Duke University

Group: B-IOME
Mentor: Babetta Marrone
Discipline: Engineering
Subject Area: Polymer and Materials Engineering

LA-UR-23-27784

DATA-ENABLED APPROACHES TO BIO-DERIVED BIOPOLYMER PROPERTY PREDICTION AND ANALYSIS

Plastics derived from petroleum are essential to life around the world, but they are detrimental to environmental and human health. Materials design of alternatives are often limited by resource-intensive experiments. In this work, we employ machine learning (ML) as a data-enabled technique to explore the structure-property relationships of a diverse family of bio-derived polyesters, poly(hydroxyalkanoates) (PHAs). A dataset was assembled to create a unique PHA degradation prediction model using ML. Varying PHA structures, degradation environments and rates, and experimental conditions were considered to explore a broad suite of variables affecting the overall degradation rate of the PHA biopolymers. An ML approach was utilized for: (1) regression for prediction of degradation rate, and (2) classification of samples into different categories of degradation profiles at specific timepoints. ML results were incorporated into the design of materials characterization analysis for PHAs and polycaprolactones to demonstrate the utility of ML-streamlined experimental polymer design.

Benjamin Laurel

Program: Undergraduate Student
School: Texas A&M University

James Phillips

Program: Undergraduate Student
School: Texas Tech University

Group: AOT-RFE
Mentor: Gabriel Cordero-Rivera

Discipline: Engineering
Subject Area: Electrical Engineering
LA-UR-23-27462

THE GLP-805 POWER SUPPLY INTERFACE

The Sorensen DC Power Supplies installed in Sector D through Sector H of the LANSCE particle accelerator, also called the 805s, are connected to the racks they sit in at four points: an AC input, a DC output, an ethernet connection, and an analog output. To perform any sort of maintenance on these power supplies, workers must go through a series of safety trainings so they can access the high voltage area at the back of the rack. Developing a new connection interface for the power supply is needed to reduce beam downtime and incorporate engineering controls to improve the safety of the power supply systems. The GLP-805 Power Supply Interface will provide a safer way for workers to access the power supplies without needing to open the high voltage area of the racks. The new interface will incorporate two separate pieces: an adapter that will mount to the power supply, and a socket that will mount to the rack. The two pieces will have a mating interface that connects each of the ports from the power supply to their respective ports on the rack.

Robert Lazarin

Program: Post-Master's Student
School: University of Texas at El Paso

Group: MPA-11
Mentor: Cortney Kreller
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27661

EVOLUTION OF DESIGN FOR HIGH PRESSURE MINIATURE FUEL CELLS

Batteries have historically been the solution for the National Nuclear Security Administration's (NNSA) small scale energy requirements. Fuel cells are being investigated as a replacement power source to support the current stockpile modernization mission. These fuel cells will be required to sit dormant for decades and, when needed, provide tens of watts of power within seconds. This is where specialized proton exchange membrane fuel cells (PEMFC's) nicknamed "Supercell" are called to action. Super-Cells are miniaturized fuel cells that operate at higher pressures than conventional PEMFC's to reduce the volume of reactant required for performance. MPA-11's super cells have been through three generations of design all focused around increasing the efficiency, decreasing mass and volume, and simplifying the manufacturing process of the stacks. This presentation will describe the evolution of the Supercell design and the ongoing efforts to increase the operating pressure to 1000psi.

Cory Liechty

Program: Undergraduate Student
School: Arizona State University

Group: ISR-1
Mentor: Ernst Esch
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27902

INCREASING PRODUCTIVITY AND SAFETY WITH A DOORSTOP

The door in a vault is required to be open while workers are performing their duties inside. The workers are required to wear hazmat gear, which drastically decreases the dexterity of the workers. Thorough research into doorstop technology revealed that none of the commercial off the shelf doorstops are suitable for a vault door. To meet ergonomic challenges as well as the requirements in a nuclear facility, a custom device to hold a vault door open was designed. The design is robust, durable, and more cost efficient than a worker holding the door. To this end, the doorstop design is lightweight, can hang from the hinge of the door, and is made of metal in order to be non-combustible. The design emphasizes the ease of manufacturing and keeps the door open 90 degrees.

Andrew Long

Program: Undergraduate Student
School: Texas A&M

Group: J-6
Mentor: Martin Tacceti
Discipline: Engineering
Subject Area: Electrical Engineering
LA-UR-23-28013

COMPARING PERFORMANCE METRICS OF INNOVATIVE VS. EXISTING SWAT DETECTION SENSORS

This project aimed to determine if a new laser motion sensor could augment the precision of an existing alignment system that uses the Stretched Wire Alignment Technique (SWAT), and currently relies on outdated and problematic IR motion sensors. To accurately compare the sensors, a mount was designed to allow the new sensor to run in parallel with the existing. This design aimed to verify the congruency of the results produced by both sensors under identical conditions. Preliminary results from the new sensor were compared to those of the existing to ascertain the improvements in precision that could be expected. Preliminary analysis shows that the newer sensor should match the data of the existing, and an improvement in precision should be observed. Based on these preliminary results, another mount will be designed for the replacement of the old sensor with the superior sensor in the SWAT stand. The implementation of this new sensor will provide improved cell alignment accuracy, and greatly simplify the alignment procedure.

Luis Luna

Program: Undergraduate Student
School: Texas A&M University

Group: E-3
Mentor: Bryan Steinfeld
Discipline: Engineering
Subject Area: Mechatronics Engineering
LA-UR-23-27770

PROOF OF CONCEPT FOR ADRESS: AGV GRIPPER, STORAGE SHELF, AND PALLET INTERFACE

The Automated Drum Retrieval and Storage System (ADReSS) project addresses a problem in the storage of hazardous material in the Transuranic Waste Facility. The current process relies on manual labor, exposing technicians to risks while mining the drums. The solution incorporates an Automated Guided Vehicle (AGV), shelf design that maximizes storage capacity, minimizes accidents, and reduces worker exposure to hazardous materials. The AGV, with height-adjustable capabilities, will autonomously navigate the warehouse and securely handle the drums mounted on specially designed pallets. This project is a proof-of-concept exploring the interface between the AGV, shelf, and pallet. This design uses a gripper mechanism mounted on the AGV to pull/push the pallet with drum off/onto the shelf. The shelves are equipped with a locking mechanism for securing the drums to the shelf. The pallets are engineered to facilitate seamless retrieval and placement using the AGV's gripper mechanism.

Mohamed Lamine Malki

Program: Graduate Student
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Group: EES-16
Mentor: Mohamed Mehana
Discipline: Engineering
Subject Area: Energy Storage
LA-UR-23-27520

OPERATE-H2: AN OPEN-SOURCE TOOL FOR OPTIMIZING UNDERGROUND HYDROGEN STORAGE

Underground hydrogen storage (UHS) is crucial in facilitating the transition to clean energy. However, efficient storage conditions require careful planning. While reservoir simulations could determine optimal storage conditions, exploring all possible scenarios is computationally prohibitive and time-consuming. Reduced-order models (ROMs) can efficiently simulate reservoir performance and analyze multiple strategies with reduced computational cost. Optimization, evaluation, and risk-assessment techniques for hydrogen energy (OPERATE-H2) is an open-source integrated assessment framework with a user-friendly graphical user interface (GUI) designed to optimize UHS operations. The GUI is developed based on high-fidelity models, ROMs, QtDesigner software, and Python programming language. OPERATE-H2 contains several functionalities, including temporal evolution to analyze UHS parameters over cycles, local and global sensitivity analysis to understand the individual impacts as well as the combined effects of geologic and operational parameters on UHS performance, and site screening feature to effectively identify the favorable sites for UHS installations.

Julian Martinez

Program: Undergraduate Student
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Group: ISR-1
Mentor: Ernst Esch
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27584

LIFTING MECHANISM FOR PIPE OVERPACK CONTAINER LID

The pipe overpack container (POC) is used within the TRUPACT-ll or HalfPACT to contain TRU waste contaminated with higher concentrations of plutonium and americium to reduce gamma exposure. The predominant challenge associated with the POC is that the lid containing the transuranic waste weighs 50 lbs., necessitating that two employees lift the lid to fill the body of the POC. This ergonomically challenging process of filling the POC results in employees having physical injuries due to lifting the POC lid for each replacement. Our team was tested to investigate this challenge and to design a lifting mechanism. Working closely with the customer, we generated a variety of design models in SolidWorks to mitigate this issue. The research, down selection, and the ultimate design are presented in this poster.

Nicholas McGrane

Program: Undergraduate Student
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Group: Q-6
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Discipline: Engineering
Subject Area: Electrical Engineering
LA-UR-23-27402

USER INTERFACE FOR THE OLYMPUS FIRING SYSTEM

The Olympus system is a modular firing system destined to be used at all LANL firing sites. Its modularity allows adding new capabilities to an existing system without the need to redesign the whole system. The Olympus system uses a touchscreen interface to control the system. This work focuses on the creation of the user interface for this system. The interface needs to be intuitive and easy to understand, while also being adaptable enough to complete complex tasks. Based on LabVIEW Object Oriented Programming, the user interface will allow easy addition of future modules.

Misael Morales

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Group: EES-16
Mentor: Mohamed Mehana
Discipline: Engineering
Subject Area: Energy Resource Engineering

LA-UR-23-27677

OPTIMAL SENSOR PLACEMENT AND MONITORING DESIGN IN GEOLOGIC CO2 SEQUESTRATION USING MACHINE LEARNING METHODS

Geologic CO2 sequestration (GCS) is considered as an important technology to reduce anthropogenic greenhouse gas emissions to the atmosphere. However, potential leakage through abandoned wellbores or natural fractures and faults pose a threat to the integrity of the stored CO2 and the surrounding environment. To ensure the safety and effectiveness of large-scale GCS, risk management and monitoring strategies are used to minimize and mitigate risks of CO2 leakage. We propose a deep a novel workflow to determine optimal sensor placement and monitoring strategy. Using a deep learning-based reduced-order model (ROM), we predict the cumulative CO2 leakage and quantify the uncertainty using a filtering-based data assimilation method. This method allows us to obtain the optimal monitoring well placement and strategy for a large-scale GCS project to ensure minimal leakage risk and optimal CO2 storage.

Ruairi O'Connor

Program: Graduate Student
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Group: XCP-8
Mentor: Eric Nelson
Discipline: Engineering
Subject Area: Aerospace Engineering
LA-UR-23-27215

STUDIES OF SPACE-CHARGE LIMITING IN CAVITIES WITH ENERGETIC ELECTRON INJECTION

A coupled electromagnetic/particle-in-cell (EM-PIC) simulation has been developed of an experimental validation platform in the EMPIRE code. The experimental platform, known as a “B-Dot” involves energetic electrons injected into a primary, 10 mm height, cylindrical cavity. The simulation explores the effects of space-charge limiting on the cavity currents. An analytic theory is derived to anticipate the response of an “ideal” cavity and compare to the behavior of the B-Dot. The space-charge limited current is expected to increase with electron injection energy per the analytic theory and this is confirmed by the EM-PIC simulations. The effect of varying injection current densities is explored for constant injection energy, with space-charge limiting of the cavity current being clearly identified in the simulation results. The effects of different injection energies on a constant injection current are also explored. Finally, some of these simulations are repeated in a 1 mm height B-Dot cavity.

Timothy Ockrin

Program: Undergraduate Student
School: Houghton University

Group: NEN-1
Mentor: Katrina Koehler
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-27778

ANALYSIS OF URANIUM DECAY ENERGY SPECTRA

Hundreds of samples a year are received at IAEA's laboratories to verify uranium and plutonium content of nuclear material. Decay Energy Spectroscopy (DES) uses high energy resolution (1–5 keV at 5 MeV) microcalorimeters to measure the alpha decays from special nuclear material. Spectral analysis of Pu, U, and other actinide DES data can be done using Decay Energy Spectroscopy Analyzer (DESA), a Python-based software. To test DESA's robustness, spectra generated with various analysis methods were analyzed and compared with certified compositions. Results from this data analysis and improvements to the DESA analysis methods are presented.

Shane Olson

Program: Graduate Student
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Group: NEN-1
Mentor: Vlad Henzl
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-28007

QUANTIFYING MATERIAL EFFECTS ON EFFECTIVE 240PU MASS

Accurate characterization of transuranic (TRU) waste is crucial for ensuring compliance with waste payload limits at the Waste Isolation Pilot Plant (WIPP). Current methods for assessing this waste at Los Alamos National Laboratory (LANL) have high uncertainties due to waste arrangement and the distribution of special nuclear material (SNM). To avoid exceeding WIPP criteria, LANL technicians intentionally underfill waste drums, resulting in increased costs, radiation exposure, and disposal time, impacting LANL's critical operations. This study aims to reduce uncertainties in calculating effective Pu-240 mass by examining different heterogeneous waste matrices. Neutron coincidence counters were used to conduct non-destructive assays on simulated waste containers with representative matrices and embedded Pu-240 sources. Various matrix geometries and compositions were simulation using MCNP. This research contributes to developing a framework for improved waste assessment using list-mode data acquisition and neutron coincidence counters.

Ashim Pandey

Program: Undergraduate Student
School: University of New Mexico

Group: AOT-RFE
Mentor: Paula Rooy
Discipline: Engineering
Subject Area: Electrical Engineering
LA-UR-23-26996

DEVELOPMENT OF NEW TEST PROGRAM TO AUTOMATE POWER METER TESTING

The Los Alamos Neutron Science Center's (LANSCE) Accelerator Operations and Technology division – Low-Level Radio Frequency (LLRF) team is developing a new LabVIEW program for system testing. The new program will automate power meter testing and calibration to enable testing and validation of power meters before deployment and provide calibration data. Automating the test procedure will make the test process more robust by increasing efficiency and quality and reducing user error while performing the calibration process. Furthermore, the new program's user interface will enable users to graphically display the test results and allow them to save the data for future or further analysis.

Owen Pannucci

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Group: NEN-1
Mentor: Tom Stockman
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-27794

IMPROVING DYNAMIC RADIATION BACKGROUND PROJECTION THROUGH INTERPOLATED CATEGORIZATION

A primary objective of Los Alamos National Laboratory is the production of thirty pits per year in the plutonium facility. DYMAC (Dynamic Material Control) is playing a pivotal role by developing in-line nondestructive material accountancy methods. Typically, background is controlled by transporting nuclear material away from a working area into a centralized measurement lab. While effective, material movement increases worker exposure, creates contamination risk, and bottlenecks production. DYMAC aims to mitigate this step, enabling more efficient inventories, near real time accounting, reduction of handling and exposure, and greater production efficiency. A necessary aspect in this methodology is taking high precision measurements of the desired radioactive material. Real time source location and strength predictions are vital for estimating dynamic background radiation. If more accurate predictions of background source locations and strengths are made, the measurements of the desired source will be more accurate as well.

Briley Perkins

Program: Undergraduate Student
School: St. Mary's University

Group: MST-8
Mentor: Joshua White
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27611

DESIGN CONSIDERATIONS FOR A HIGH TEMPERATURE LOAD FRAME FOR CREEP TESTING OF NUCLEAR FUELS

Nuclear reactor fuel rods are composed of cylindrical ceramic uranium oxide pellets that are contained within alloyed zirconium rods. Current industry initiatives are replacing traditional UO2 pellets with doped UO2 variants to improve the fission gas release characteristics as well as improve the thermomechanical creep behavior in-pile. However, the existing creep databases have not accurately described the behavior over all relevant reactor conditions, which requires further investigation. The purpose of this project was to design and implement a Radio-Frequency furnace to enable high temperature compression testing on advanced ceramic fuel forms. We used the iterative design process through computer aided design software to design an air tight thermomechanical creep rig to measure properties to <2000°C. The design process utilized 3D printed parts to rapidly prototype the design and improve upon the furnace. Preliminary testing of the RF furnace design was performed to monitor temperature stability.

Jacob Petersen

Program: Undergraduate Student
School: University of Tennessee, Knoxville

Group: P-4
Mentor: Eric Loomis
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-28022

DOUBLE SHELL INERTIAL CONFINEMENT FUSION X-RAY SPECTRAL ANALYSIS

At the National Ignition Facility (NIF), lasers are used to compress a double shell capsule with deuterium and tritium in order to create nuclear fusion processes. The lasers aim at the inside of a gold hohlraum which excite electrons which further release photons in the range of 0~20keV. 'Dante' analyzes this data by having 18 planar vacuum x-ray diodes (XRD) behind unique filters to differentiate data amongst various photon energies. The goal of the project was to analyze the characteristics of low and high energy photons released by the gold shell.

Lalith Sai Srinivas Pillarisetti

Program: Graduate Student
School: Pennsylvania State University

Group: MPA-11
Mentor: Eric Davis

Discipline: Engineering
Subject Area: Ultrasonics
LA-UR-23-27659

NON-INVASIVE FLUID LEVEL SENSING IN PIPELINES USING ULTRASOUND TECHNIQUES

Accurate assessment of waste detection in sealed pipe systems is crucial in waste-water treatment and petrochemical plants. The traditional pulse-echo time-of-flight measurements using ultrasound sensors to measure the fluid level are challenging for low fill levels due to signal contamination with multiple echoes and the resonances in the pipe wall. In this work, we identify the challenges induced by the resonances within the pipe and propose numerous strategies to improve pulse-echo measurements, such as employing a narrow bandwidth pulse, appropriate filtering away from the resonance frequencies, and baseline subtraction. We also propose a resonance-based ultrasonic technique that is highly sensitive to fluid levels. However, the pulse-echo and resonance techniques demand precise calibration with the pipe system before use. To mitigate the need for calibration, we propose a phased array imaging technique based on the total focusing method to facilitate better visualization of the fluid level up to low fill levels.

Roshan Prasad

Program: Undergraduate Student
School: Texas A&M University

Group: W-11
Mentor: Eric Raynor
Discipline: Engineering
Subject Area: Mechanical and Systems Engineering
LA-UR-23-27551

DESIGNING POWER SYSTEMS FOR FLIGHT TELEMETRY: MECHANICAL AND SYSTEM REQUIREMENTS

In harsh environments, sensor networks their DAQ's and their power distribution systems need robust housing and shielding. While many sensors are rated for high temperatures and loading, battery cells are often not as robust. Therefore, proper design of battery housing needs to include RF/EMF shielding, proper thermal dissipation, force absorption and vibration damping. Design for housing must consider each of these aspects and should be validated with engineering analysis. In addition, implementation and tooling must be considered in the design process. There are multiple solutions for a container with these qualities and comparison of different designs relies upon intensive thermal and structural analysis. Three such designs are proposed, and their performance are documented.

Taylor Quintana

Program: Undergraduate Student
School: New Mexico State University

Group: AOT-MDE
Mentor: Walter Barkley
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27365

PORTABLE WATER FLUSH CART REDESIGN AND DETAIL

There are two Water Flush Carts frequently used at Los Alamos Neutron Science Center (LANSCE), identical when purchased in the early 2000s. One is primarily used throughout the particle accelerator to flush out components water cooling systems that have debris blocking normal flow. The other one is primarily used for testing components and systems that are being fabricated at LANSCE. These carts have had parts replaced many times by different teams throughout the years for maintenance and improvements, causing them to differ from the original design they had. To improve flow rate and make the carts identical once again, I have redesigned the plumbing and frame. Using SolidWorks CAD, I worked with various teams at LANSCE to improve the design per their suggestions. I created assembly drawings including a Bill of Materials to further assist with purchasing the new components and fabrication. The parts are currently in the process of being ordered and once they arrive, the new carts can begin to be built. The focus of this poster is the modeling process in Solidworks and the reason behind the updates and layout changes I added to the overall design/layout.

Jackson Rahm

Program: Undergraduate Student
School: Texas A&M University

Group: W-11
Mentor: Skyler Addams
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27550

CONTINUOUS CARBON FIBER-PEEK 3D PRINTING HOT-END

Developing additive manufacturing methods for thermoplastic-coated carbon fiber will substantiate development of future graphite-coated carbon fiber processes to enhance agile capabilities relative to nuclear stockpile stewardship. A proposed solution is to design a 3D-printer hot-end block capable of sustaining a temperature of 450 ^{o}C while coating the carbon fiber in PEEK thermoplastic. Such a design is further bound by making use of existing 3D-printing hardware. Furthermore, an optimal design feature is to allow disassembly for cleaning and future development. To function at high temperatures, the block is constructed from Aluminum Bronze, chosen for its high annealing temperature and thermal conductivity. To mix the carbon fiber and thermoplastic, an internal channel and reservoir are added to the block. A removable lid is also integrated to make these components accessible. This proposed design considers manufacturability, heat transfer, material properties, and existing size requirements to meet the given constraints.

Maheen Rahman

Program: Undergraduate Student
School: Texas Tech University

Group: AOT-IC
Mentor: Heath Watkins
Discipline: Engineering
Subject Area: Electrical Engineering
LA-UR-23-27740

LANSCE'S LINAC CONTROL UNIT CHASSIS

Develop a prototype intended for the management of the control network of the Los Alamos Neutron Science Center's (LANSCE) linear particle accelerator (LINAC) using USB or smart knobs, toggle switches, push buttons, and an integrated screen. With a focus on enhancing the user experience, the project incorporates haptic and visual feedback features.

Rebeca Rocha

Program: Undergraduate Student
School: Texas A&M University

Group: E-6
Mentor: Christina Hanson
Discipline: Engineering
Subject Area: Non-Destructive Testing and Evaluation
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 am 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.

Andrew Ruba

Program: Post-Bachelor's Student
School: Iowa State University

Group: MPA-11
Mentor: John Matteson
Discipline: Engineering
Subject Area: Chemical Engineering
LA-UR-23-27663

DESALINATION VIA PERVAPORATION TO ENABLE WATER RECOVERY FROM PRODUCED WATER

Over one trillion gallons of produced water, brackish water, and brine water was produced as a byproduct of oil and gas extraction in 2021. These solutions have total dissolved salt (TDS) levels generally ranging from 3,000 mg/L to 300,000 mg/L and contain varying degrees of hydrocarbons or organic compounds, making water treatment difficult and energy intensive. In this work, a highly selective polybenzimidazole (PBI) thin film pervaporation membrane was evaluated for desalination of high TDS solutions for water recovery applications. Conductivity measurements of treated water range from 12.3 µS/cm to 32.3 µS/cm, which shows exceptionally high salt rejection rates. UV-Vis spectroscopy shows a 99.9% organic rejection rate, which is not well documented in literature. This work outlines a promising path forward of scaling this technology for the treatment of high TDS solutions.

Christian Ruiz

Program: Graduate Student
School: University of Texas at El Paso

Group: MPA-11
Mentor: Tommy Rockward
Discipline: Engineering
Subject Area: Materials Science and Mechanical Engineering
LA-UR-23-28113

ULTRASONIC NON-DESTRUCTIVE EVALUATION OF ADDITIVELY MANUFACTURED POLYMER-CERAMIC PARTS

Digital light processing (DLP) is an attractive additive manufacturing technique due to its ability to create ceramic parts with complex geometries. DLP uses ultraviolet light to polymerize a slurry comprised of ceramic powder and photosensitive resin in layers to create solids parts. Printing parameters such as light intensity and exposure time are critical when producing these parts. Incorrectly choosing parameters can lead to over-or under-curing, which negatively effects both the print quality and strength. The aim of this research was to investigate the effect of printing parameters on the ultrasonic response of alumina polymer-ceramic composite parts. Samples were printed at varying layer exposure times while observing the acoustic velocity through the sample and comparing it with a validation matrix. The print parameters are directly correlated with the ultrasonic response allowing the optimal exposure to be determined.

Juan Sanchez

Program: Post-Bachelor's Student
School: University of Central Florida

Group: XCP-2
Mentor: Robert Pelak
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-28041

RESOLVING HYDROCODE ASYMMETRIES AND AN EXPLORATION OF PROGRAMMED TO REACTIVE BURN MODEL INTERACTIONS

Studies performed in the Summer of 2022 showed asymmetries when modeling the effects of the underground detonation of a conventional High Explosive (HE). Asymmetries in the Eulerian Hydrocode PAGOSA are demonstrated in plots of shock wave pressure, and size of the cavity produced with time. The source of the asymmetries were traced to the use of a value of detonation velocity that was lower than the Chapman-Jouguet velocity, as the result of a bug involving confusing variable names. In the second part, transition from a programmed burn to a reactive burn model is explored in copper cylinder test simulations to test my new implementation of the WSD (Wescott-Stuart- Davis) reactive burn model in PAGOSA. Detonation of a cylindrical pellet of 9501, modeled with a program burn, is used to detonate a cylinder of 9502, modeled with WSD, and plots generated are compared to experimental tests.

Anisha Selvan

Program: Undergraduate Student
School: Texas A&M University

Group: E-14
Mentor: Sandra Zimmerman
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27254

EVALUATING DIGITAL IMAGE CORRELATION AS AN ALTERNATIVE TO TRADITIONAL MODAL TESTING MEASUREMENT METHODS: A FURTHER UNDERSTANDING OF CURRENT ADVANTAGES AND LIMITATIONS

Modal testing aims to determine structural modal parameters: natural frequencies, damping coefficients, and mode shapes. This is crucial in the establishment of design requirements for systems needing to withstand varying environmental conditions. With the prominence of multi-axial excitation modal tests, it is important that full-field measurements be captured, while minimally affecting the test object's behavior. Thus, enabling the understanding of test structure geometry and characterization of vibrational behavior under stress. With sensor-based modal testing, data can only be collected from the point at which sensors are placed. Digital image correlation (DIC), a technique which measures surface displacement across a test object through the tracking of rapidly captured image sequences, poses a possible advancement from current modal testing techniques. This work evaluates the effectiveness of DIC techniques and correlation analysis in the recording of a box assembly with removable component (BARC) structure's resulting mode shapes from a multi-axial excitation modal test.

Gabriel Serrano

Program: Undergraduate Student
School: University of New Mexico

Group: P-4
Mentor: Tana Morrow
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27389

MECHANICAL DESIGN AND FABRICATION OF A FOIL HOLDER FOR A LASER DRIVEN X-RAY SOURCE

The Laser Driver Source (LaDS) is being developed to evaluate current P-4 diagnostics and future X-ray, Neutron, and Gamma diagnostics for remote facilities. The Diagnostics and Operations Engineering team aims to create a laser-driven x-ray source that delivers high-intensity, pulsed characterization for these diagnostics. The mechanical design objective focuses on developing a foil holder to accommodate various compositions and thicknesses of foil targets. This holder needs to be attached to a vacuum interface Linear Bellows Drive, which positions a foil in the laser's path, enabling the desired operation of the source. The final design consists of a 4" x 1.5" x 1/8" metal frame with three 1" holes, allowing attachment of multiple foil types using adhesive. This presentation will discuss the mechanical design and fabrication process of the foil holder frame.

Emerson Shands

Program: Graduate Student
School: Texas A&M University

Group: CCS-2
Mentor: Mario Ortega
Discipline: Engineering
Subject Area: Nuclear Engineering
LA-UR-23-27889

GALERKIN QUADRATURE METHODS IMPLEMENTED IN PARTISN

Two methods, GQ2 and GQ3 (Galerkin Quadrature), for representing the scattering source of the Boltzmann neutron transport equation were implemented in the LANL neutron transport code PARTISN. These methods expand upon the hybrid collocation-Galerkin-Sn method introduced by Dr. J. Morel. The aim of these methods was to accurately describe and approximate highly anisotropic delta function scattering. The original PARTISN implementation was expanded to include the two new methods, and all three were compared against a reference test problem.

Kassidy Shedd

Program: Graduate Student
School: Northwestern University

Group: MPA-Q
Mentor: Nicholas Dallmann
Discipline: Engineering
Subject Area: Signal Processing
LA-UR-23-27948

CLUTTER SUPPRESSION AND TARGET ISOLATION USING RADAR SIGNAL PROCESSING

Moving target detection in a 3D space using transmitter-receiver radar signals is made difficult by background clutter caused by stationary objects in the observation region. Frequently, the target will get lost in the background clutter and noise, making the target indistinguishable amongst these features. This project aims to address this issue by using 1- and 2-dimensional interpolation methods to align sequential frames and thereby eliminate common characteristics such as the direct path (an uninterrupted transmitter-receiver radar path) and background clutter. This project uses python and scipy.interpolate libraries to perform interpolation. The goal of this project is to be able to make a moving target identifiable amongst other features present.

Reid Stradling

Program: Undergraduate Student
School: Brigham Young University

Group: W-11
Mentor: Paul Romo
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27801

LITHIUM BATTERY CHEMISTRIES

I will be presenting on different types of lithium battery cells that can be used in a specific application within a closed system. This system will include sensors and the heat output from the batteries needs to be measured and controlled. I will look in-depth at lithium titanate, lithium iron phosphate, and lithium nickel manganese cobalt oxide batteries. I will compare safety and performance factors in each. I will also give a broad overview of battery chemical properties and characteristics.

Aleck Tilbrook

Program: Undergraduate Student
School: Liberty University

Group: E-14
Mentor: Peter Fickenwirth
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-26356

IMPROVED SHAKER CAPABILITY ESTIMATION THROUGH OUT-OF-AXIS MOTION MODELING

The objective of this work is to use frequency based substructuring to predict the electrical requirements needed by an electrodynamic shaker to achieve a given test specification for a device under test (DUT). Electrodynamic shakers are commonly used pieces of equipment considered by many to be vital for the purpose of environmental shock and vibration testing. However, the capabilities of these shakers can be influenced by the dynamic coupling between the shaker itself and the DUT being utilized. The coupled dynamics between the two has the potential to introduce difficulties when attempting to achieve desired excitations. Characterization of the coupled dynamics is necessary for determining test feasibility in these instances. This work seeks to improve upon a previous model of an electrodynamic shaker by increasing its complexity with the introduction of the shaker's out-of-axis motion.

Lyra Troy

Program: Post-Master's Student
School: University of Arizona

Group: C-CDE
Mentor: Joseph Dumont
Discipline: Engineering
Subject Area: Chemical Engineering
LA-UR-23-27953

EVALUATION OF HYDROGEN PERMEATION FOR THE DIRECT INTERNAL RECYCLE (DIR) CONCEPT IN THE FUSION FUEL CYCLE

Nuclear fusion could provide an unlimited source of clean energy using hydrogen isotopes, Deuterium (D) and Tritium (T), as fuel. In the Fusion Fuel Cycle, D-T mixtures are sent into a fusion reactor with a fuel burnup fraction of ~5% to produce energy. The remaining 95% of unreacted D-T fuel is delivered through extensive processing stages before returning to the reactor, equating to increased time and cost. The Direct Internal Recycle (DIR) system is a proposed concept to reroute fuel directly back into the reactor, effectively reducing processing steps and tritium inventory, subsequently lowering costs. Data from unit operations, such as permeators, is required to validate and refine the DIR concept. In this work, experimental data will be provided from the Hydrogen Processing Laboratory (HPL) using hydrogen as a surrogate for tritium. The performance of hydrogen permeation will be evaluated as a function of hydrogen concentration, flow rate, and temperature.

Albert Wen

Program: Graduate Student
School: University of California San Diego

Group: E-1
Mentor: Alessandro Cattaneo
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27362

RFID TAG MOUNT DESIGN FOR NUCLEAR MATERIAL CONTAINERS

Nuclear material inventory accounting at Los Alamos National Laboratory (LANL) could benefit from the adoption of modern inventory systems. As demonstrated in a wide variety of industry scenarios (e.g., manufacturing, retail, distribution), radio frequency identification (RFID) technologies have been successfully utilized to expedite accounting for assets and reduce risk of error. An ongoing effort at LANL is addressing the technical and administrative challenges posed by the adoption of RFID technologies for nuclear material control and accountability. Tests performed last year with SAVY and slip-top containers and commercial off the shelf (COTS) handheld RFID technology have revealed the need for RFID tag mounts that meet the following design objectives: 1) protect the side-mounted RFID tags from damage and/or tampering, 2) withstand handling while remaining fixed to the containers, 3) avoid compromising container integrity, 4) maintain sufficient spacing between containers to ensure RFID tag performance, and 5) minimize mechanical changes to the user experience (e.g., compatibility with existing processes). This work proposes combining computer-aided design (CAD), finite element analysis (FEA), and 3D printing to develop effective tag mounts. Simulations and physical experiments will inform the iterative design process to arrive at a functional tag mount that best meets the objectives.

Jason Wilkening

Program: Graduate Student
School: Purdue University

Group: M-9
Mentor: William Perry
Discipline: Engineering
Subject Area: Mechanical Engineering

LA-UR-23-27579

DEFLAGRATION AT EXTREME PRESSURES

The SURF continuum reactive burn model takes a novel approach to predicting the shock sensitivity of explosives which accounts for material microstructure. In this model, a shock causes the formation of burn centers which have an associated surface area over which an initial deflagration occurs. In this model, a critical parameter in describing the shock-dependent build-up to detonation is the pressure sensitivity of this initial deflagration reaction, which is currently characterized phenomenologically (using experimental data) via Vieille's law. In this work, we leverage some classic deflagration models, including the Dennison-Baum-Williams, Ward-Son-Brewster, and Beckstead-Derr-Price solid propellant deflagration models to make quantitative predictions of the deflagration speed from basic material physicochemical properties. The application of these models introduces myriad physically meaningful sensitivities to the shock initiation of explosives, including decomposition kinetics, thermal conductivity, and initial temperature, marking an important step forward in the predictive modeling of explosive shock response.

Emily Wong

Program: Undergraduate Student
School: Texas A&M University

Group: PFE-GB
Mentor: Renee Mondragon
Discipline: Engineering
Subject Area: Mechanical Engineering
LA-UR-23-27684

BUBBLER OIL VISCOSITY EXPERIMENTAL DESIGN

Pressure relief devices, commonly known as bubblers, are used in glovebox systems to maintain inert atmosphere inside the gloveboxes. Recently, a new oil was introduced to these bubblers; however, this oil was observed to disappear more rapidly than previous oils used. Additionally, this oil was found to travel outside of the bubbler and into the ventilation system or gloveboxes. This unwanted distribution of oil could be due to properties of the new oil or excessive purging of gas. It is believed the viscosity of oil contributes most to oil travelling outside the bubbler. In this procedure, the testing requirements, materials, methodology, and measurements are defined to test a range of silicone-based oils with varying viscosities. The aim of this procedure is to develop a method for determining which oil depletes the slowest and stays bubbling within the base of the bubbler while maintaining an acceptable range of pressures.

David Yapell

Program: Graduate Student
School: Florida International University

Group: MPA-11
Mentor: Tommy Rockward
Discipline: Engineering
Subject Area: Computer Engineering
LA-UR-23-27792

PROBING THE CORROSION RATES OF NOVEL TITANIUM SUBSTRATES IN A SIMULATED PEM FUEL CELL ENVIRONMENT

Metallic bipolar plates are often used in proton exchange membrane fuel cells (PEMFCs) due to their facile manufacturing process, high electrical and thermal conductivity, and mechanical strength. Titanium is particularly popular due to its corrosion-resistive properties which come from a naturally occurring passive oxide layer on its surface. However, the naturally occurring passive film cannot fully withstand the acidic environment of an operating PEMFC. And inherently, without this protective layer; corrosion will inevitably occur. In this study, the corrosion resistance of commercially pure titanium with thermally grown oxidation layers and titanium directly coated with a commercial sub-oxide coating was investigated. The corrosion resistance of the various samples were examined with potentiostatic and potentiodynamic tests in sulfuric acid solution at various temperatures to simulate PEMFC conditions. The samples were also subjected to a novel accelerated stress test to evaluate long term durability under fuel cell vehicle startup and shutdown conditions.

Julie Young

Program: Undergraduate Student
School: University of Nevada, Reno

Group: PFE-CV
Mentor: Eric MacFarlane
Discipline: Engineering
Subject Area: Earthquake Engineering
LA-UR-23-28239

PROCESSING SEISMIC RESPONSE SPECTRA

My project is a virtual presentation on what seismic response spectra is and how to process it.

Health and Safety

Alfredo Cortez

Program: Post-Master's Student
School: Texas A&M University

Group: RP-PROG
Mentor: Jordan Douglas
Discipline: Health and Safety
Subject Area: Health Physics
LA-UR-23-27748

EFFECTS OF BREMSSTRAHLUNG RADIATION OPTIONS ON DOSE CALCULATION IN MCNP6.3

This project focuses on electron transport in MCNP6.3 and how to use different options to speed up run times while keeping the results valid for both high and low energy electrons. The low energy electrons were tested with a model of a 160 KeV X-ray tube. The high energy electrons were tested using a model of a LINAC with 5 MeV electrons. There was a total of four options used. The first was the BBREM card which was used to bias bremsstrahlung production. The second is the electron physics card used to turn on and off knock-on electrons. The third is the DBCN card used to modify the energy-indexing algorithm of electron transport. The final method is a commonly used technique of using electron cut-off energies.

Elise Olivas

Program: Undergraduate Student
School: New Mexico State University

Group: OSH-DS
Mentor: Dana Brake
Discipline: Health and Safety
Subject Area: Occupational Safety
LA-UR-23-28149

EXOSKELETONS: AN ANALYSIS OF OCCUPATIONAL SAFETY AND THE RISK REDUCTION OF MUSCULOSKELETAL DISORDERS

Work-related musculoskeletal disorders (WMSDs) occur when the duration and severity of exposure to ergonomic stressors accumulate over time, placing high levels of physical demand on the human body. These stressors may consist of manual lifting, upper extremity repetitive motion, and awkward postures. To flatten the curve of these injuries, the use of exoskeletons is one example of an engineered solution that has been increasingly researched. Although exoskeletons have only been seriously researched for less than 10 years, the CDC determined that the use of these wearable robotics can potentially assist workers in reducing their exposure to the physical demands of work through mechanical interaction with the body. Now, groups at Los Alamos National Laboratory are deploying these devices into the field to provide additional research as a part of a nationwide effort to better understand their effectiveness, all in collaboration with Ergonomics and Industrial Hygiene & Safety.

Materials Science

Allen

Program: Post-Bachelor's Student
School: Florida Agricultural and Mechanical University

Group: MPA-11
Mentor: Tommy Rockward
Discipline: Materials Science
Subject Area: Electrochemistry
LA-UR-23-27819

INK PARAMETRIZATION FOR SLOT-DIE ELECTRODE MANUFACTURING

The emergence of fuel cells and electrolyzers into the commercial market opens doors for new manufacturing processes. The production of fuel cell components will have to keep up with the forecasted growing demand. One of the major components are the electrodes, anode and cathode. The electrodes consist of an electrocatalyst deposited onto a gas diffusion layer (GDL) to facilitate the hydrogen oxidation reaction (HOR) and the oxygen reduction reaction (ORR) to produce electricity. Here we propose using a slot-die coater as an electrode manufacturing technique. This technique can produce higher volumes when compared to other methods by depositing electrocatalyst in thin and uniform films with minimal material waste and low operational cost. Our focus is to overcome the challenges associated with this manufacturing technique (e.g. electrode uniformity, catalyst suspension, and ink viscosity. X-ray Fluorescence is used to perform elemental mapping and gauge the uniformity.

Zachary Barker

Program: Graduate Student
School: University of Texas at El Paso

Group: MST-16
Mentor: Meghan Gibbs
Discipline: Materials Science
Subject Area: Metallurgical and Materials Engineering

LA-UR-23-27639

EXPERIMENTALLY DETERMINED HEAT TRANSFER COEFFICIENTS

The heat transfer coefficient (HTC) is an integral property of material interfaces in heat transfer systems. It is dependent on many other variables, including temperature, interface material, coating, surface finish at interface, and atmosphere. The lack of a database to pull these values from has required modelers to resort to guesses. Thermocouples were placed near the interface between two graphite blocks. A Labview program was used to pull and evaluate TC data into temperature. Temperatures were taken at 400 oC and 200 oC, in as close to a one-dimensional steady state problem as possible. From there, temperatures at the interface were estimated by fitting a polynomial function to the data and the heat flux across the interface was established from those temperatures. A table of HTCs were obtained using parametric analysis of the surface finish roughness. These values were found to compare to those obtained from tuned models.

Tinsley Benhaddouch

Program: Graduate Student
School: Florida International University

Group: MPA-11
Mentor: Cortney Kreller
Discipline: Materials Science
Subject Area: Electrical Engineering
LA-UR-23-27100

DIELECTRIC PROPERTIES OF LANTHANIDE RARE EARTH OXIDES

Gate oxides for beyond-silicon microelectronics require specific dielectric properties and Lanthanide Rare Earth Oxides are being explored for their suitability in such applications. Lanthanide series oxides are also predicted to form a variety of crystalline phases. Changes between these phases could affect the functional dielectric properties. Experimentally validating this phenomenon contributes to our group's overarching efforts to elucidate the associations between structural properties and functional properties of these oxides. A structured approach requires 1) pre-characterization of the 'as fabricated' oxides, 2) means to promoting the phase change, and 3) post-characterization. Exposure to light-ion irradiation induces phase changes in these materials. The pre and post characterization regimen highlights Ellipsometry as the technique to extract the complex index of refraction and complex dielectric functions to ultimately track the changes of the optical and dielectric properties in the material. This presentation reports upon our ongoing efforts and gives insight into its future direction.

Thai hang Chung

Program: Graduate Student
School: Bowling Green State University

Riley Ferguson

Program: Graduate Student
School: Bowling Green State University

Group: MST-8
Mentor: Yongqiang Wang
Discipline: Materials Science
Subject Area: Physics
LA-UR-23-27662

IN-SITU POSITRON ANNIHILATION SPECTROSCOPY

As one of the thrusts of the DOE Energy Frontier Research Center (EFRC) Fundamental Understanding of Transport Under Reactor Extremes (FUTURE), we are pioneering the development of an in-situ positron annihilation spectroscopy (iPAS) beamline to enable a pillar of the Center: designing new capabilities to quantify the fundamental mechanisms behind the early stages and evolution of non-equilibrium defects as they are exposed to the demanding operating environments found in nuclear. iPAS is a pulsed non-destructive 30keV positron probe capable of depth-resolved measurements of defects with atomic-scale sensitivity. The beamline target chamber is coupled to a heavy ion 3 MV tandem accelerator for in-situ monitoring of ion displacement damage production allowing us to monitor the time evolution of transient vacancy defects and vacancy clusters. Currently, upgrades include optimization of the buncher, an updated ion beam monitoring system, and an active magnetic field cancellation for field fluctuation compensation.

Mack Cleveland

Program: Graduate Student
School: Massachusetts Institute of Technology

Group: Sigma-2
Mentor: Robert Hackenberg
Discipline: Materials Science
Subject Area: Materials Informatics
LA-UR-23-27777

MATERIALS DATA EXTRACTION WORKFLOW

The ever-growing amount of materials science literature requires makes it impractical to digest the entirety of materials science research. Databases that allow for programmatic querying of articles based on conceptual tags help address this problem, but databases are inconsistent in how they report materials composition. To overcome this limitation of databases, we designed an automated workflow to extract material compositions from unstructured texts including pdfs, or xmls. After practicing with a curated library of metallurgy literature, we identified common and accessible syntaxes authors use to report their materials' compositions. We developed a method to extract compositions for likely materials and identify the presence of elements. Our results show what materials composition spaces have been explored and contribute a tool to the burgeoning field of materials informatics.

Sean Drewry

Program: Graduate Student
School: University of Tennessee, Knoxville

Group: MST-8
Mentor: Scarlett Widgeon Paisner
Discipline: Materials Science
Subject Area: Nuclear Materials
LA-UR-23-27609

PERFORMANCE AND PROPERTIES OF CR-UO2 FUEL FOR LIGHT WATER REACTORS

Select metallic oxide dopants have been added to UO2 to increase grain growth during sintering for accident tolerant fuels in light water reactors (LWRs). For this study, chromia (Cr2O3) is added in concentrations ranging from 750-7800 ppm to UO2 and sintered at 1750 °C for 8 hrs. Increased grain size promotes the retention of fission products within the grains and increases fuel pellet plasticity. Densities will be measured through geometric calculations. The Cr-doped UO2 microstructure will be investigated by scanning electron microscopy and energy dispersive x-ray spectroscopy (SEM-EDXS) to determine average grain size and elemental distribution of Cr in the UO2 matrix. Slight changes to the lattice parameter (a) due to Cr incorporation in the UO2 lattice are determined by X-ray diffraction (XRD) and refined through Rietveld refinement of XRD patterns. Thermophysical properties will be measured to understand the effects of Cr dopants on the UO2 bulk behavior.

Zhangxi Feng

Program: Graduate Student
School: University of New Hampshire

Group: MST-8
Mentor: Daniel Savage
Discipline: Materials Science
Subject Area: Mechanical Engineering
LA-UR-23-27701

MILKING THE HIPPO - AUTOMATED APPROACH TO BATCH RIETVELD REFINEMENT

The MAUD Interface Language Kit (MILK) is a Python package consisting of a set of Rietveld analysis tools for automated processing of diffraction datasets. By default, it interfaces with the Material Analysis Using Diffraction (MAUD) program but can be adapted for other software such as GSAS-II. The main features of MILK are to ensure programmable and reproducible Rietveld refinements, enable parallel computing capabilities, provide refinement summary, organize and build database of the data and analysis results, and visualize the results using other publicly available packages. The main work done here is to prepare MILK for public distribution and encourage the diffraction community to learn and use it to accelerate the Rietveld processes. Any user interested can download MILK from the GitHub (github.com/lanl/milk) and follow the Wiki tutorials.

Alyssah Fuentes

Program: Undergraduate Student
School: University of Texas Rio Grande Valley

Group: MPA-11
Mentor: Bianca Ceballos
Discipline: Materials Science
Subject Area: Materials Synthesis
LA-UR-23-28283

EFFECTS OF APTES CONCENTRATION ON THE MORPHOLOGY AND HYDROGEN PERMEATION OF PD THIN FILM MEMBRANES

Palladium thin film membranes have shown success in separating hydrogen from gaseous compounds for energy storage. This study aims to improve the functionality of these membranes with the use of an intermediary layer in the form of (3-Aminopropyl)triethoxysilane (APTES). The addition of palladium diacetate trimer ([Pd(OAc)2]3) provides dual seeding of Pd on the film with electroless plating method providing primary seeding. Characterization of the samples suggests the use of [Pd(OAc)2]3 with APTES increases the deposition of Pd onto the fiber. Utilizing a dual seeding method in the second set of experiments yields a homogenous Pd thin film growth with few defects.

Quinton Geller

Program: Undergraduate Student
School: University of Pennsylvania

Group: MST-8
Mentor: Donald Brown
Discipline: Materials Science
Subject Area: Materials Science
LA-UR-23-27435

MODELING THE BIPHASIC THERMAL DEFORMATION OF ALPHA AND DELTA PLUTONIUM

Of plutonium's allotropes, δ-Pu is of primary interest for nuclear application due to its highly symmetric, face-centered cubic structure. While gallium stabilizes it across a wide temperature range, it nonetheless gradually transitions into the simple monoclinic α phase at low temperatures. To better characterize the mechanical relationship between these phases, biphasic finite element models with (1) laminar, (2) concentric cubic, and (3) interpenetrating geometries were created in ABAQUS and subjected to a uniform temperature decrease from 300 K to 10 K. Each was constructed as a representative volume element, and the stress and strain in each phase was determined as a function of temperature. The resulting plots were compared to experimental results from the Advanced Photon Source in 2021.

Adrian Gonzales

Program: Graduate Student
School: University of Texas at San Antonio

Group: MST-8
Mentor: Joshua White
Discipline: Materials Science
Subject Area: Nuclear Fuels
LA-UR-23-27062

CHARACTERIZATION OF HYDROGEN INTERACTION WITH HIGH-DENSITY FUELS

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. Typical oxidation characterization involves using XRD and SEM images which can be difficult in detecting hydrogen absorption. 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.

Marcos Hernandez

Program: Graduate Student
School: University of New Mexico

Group: C-CDE
Mentor: Joseph Dumont
Discipline: Materials Science
Subject Area: Materials Science
LA-UR-23-27047

IR SPECTROSCOPY OF BACTERIAL METABOLIC UTILIZATION FOR PATHOGENIC IDENTIFICATION

Methods for rapid identification and response to hazardous pathogens, such as Escherichia coli and Salmonella, are essential to limiting and monitoring the spread of harmful bacterium. However, current bacterial identification techniques require direct interaction with the sample, leading to exposure risks for researchers. Furthermore, the lack of comprehensive spectral libraries limits capabilities for the remote detection of biological threats. By taking IR spectral measurements of the unique metabolic profiles of bacterial strands (i.e. fermentation of glucose, lactose, glycerol), these signatures may be used to identify pathogenic vs. non pathogenic bacteria and distinguish pathogens from their surrounding environments. By analyzing the growth media following growth of the bacterium (spent media), the consumed media components needed for growth will allow for the identification of specific bacterial strains. From this library of unique spectral fingerprints, we look to develop a biochemical spectroscopy tool for identifying bacterial pathogens based on their unique metabolic profile.

Minhtet Htoon

Program: High School Student
School: Los Alamos High School

Group: MPA-CINT
Mentor: Benjamin Derby
Discipline: Materials Science
Subject Area: Materials Testing
LA-UR-23-27453

AUTOMATION IN MATERIALS TESTING

Mechanical testing of materials helps to keep people, structures, and the planet safe. With the advent of computers and robots, automated mechanical testing of materials like steel and concrete has become standard in industry for many decades and has helped develop new materials faster. Unfortunately, this type of automation has not taken a hold in research environments. This presentation will go over what integration of a robot in a R&D materials testing lab looks like and showcase the problems needed to be solved for R&D automation. These are based of our experience integrating a robot into an existing R&D material testing system at Los Alamos National Laboratory, inspired by existing industrial solutions for automating materials testing. Although primarily intended for materials testing, some of the more general suggestions in this presentation could be used in other fields of research looking to automate testing.

Genevieve Kidman

Program: Graduate Student
School: University of Nevada, Las Vegas

Group: Sigma-2
Mentor: Daniel Hooks
Discipline: Materials Science
Subject Area: Mineral Physics
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 nonloaded 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.

Victoria Kwei

Program: Undergraduate Student
School: University of New Mexico

Group: MPA-11
Mentor: Tommy Rockwood
Discipline: Materials Science
Subject Area: Materials Engineering
LA-UR-23-27486

OPTIMIZING MINIATURE HYDROGEN FUEL CELL STACKS

The 2B hydrogen fuel cell stack is designed to operate over a broad range of temperatures, from sub-zero to 80°C. Most matter shrinks at freezing temperatures and expands at higher temperatures, so it is critical to use materials that can withstand large variations while maintaining a gas tight seal. We are evaluating different gasket materials and configurations of the end-plates with springs to see which combination has the least amount of pressure loss under thermal cycling. We are also testing different catalysts for the best performance. We are looking at different platinum catalyst powders that have different crystallite sizes and loadings on the electrode, which can affect the reaction rate. The data collected and information learned through this project will help add input to the design of 2B stack. Our aim is to provide a power source that can operate consistently from Antarctica to the Sahara Desert.

Joseph Leal

Program: Undergraduate Student
School: Texas A&M University

Noah Pearlstein

Program: Undergraduate Student
School: Purdue University

Group: MST-16
Mentor: Zachary Levin

Discipline: Materials Science
Subject Area: Materials Science and Engineering
LA-UR-23-27608

AN INVESTIGATION OF NANOINDENTATION AS QUALITY CONTROL

Nanoindentation is an important tool in the rapid testing of materials for quality control. With changes in the material properties due to altered chemistry and processing, and the increasing risk of receiving counterfeit items, parts may have a wide variance in quality. As such, it is important to test the materials properties that are required by the specification to ensure they function as intended in-service. Nanoindentation can rapidly perform thousands of indents upon a surface automatically. The large scale maps the indenter generates can be used to visualize and record values such as hardness and modulus without the need for traditional mechanical testing, which is time-consuming, more destructive, and uses larger quantities of material. The indenter can also perform more specialized experiments, such as strain rate jump testing and fatigue testing to further characterize behavior. Ultimately, nanoindentation is an important tool for the rapid testing of materials for quality control.

Sangwon Lee

Program: Graduate Student
School: University of Michigan

Group: MST-8
Mentor: Reeju Pokharel
Discipline: Materials Science
Subject Area: Materials Science Engineering
LA-UR-23-27795

3D IN-SITU MICROSTRUCTURE CHARACTERIZATION OF TIN USING HIGH-ENERGY X-RAY DIFFRACTION MICROSCOPY

High-Energy Diffraction Microscopy (HEDM) is a powerful non-destructive characterization technique that provides valuable insights into the crystallographic properties of materials. In this study, we investigate the microstructural behavior of Tin (Sn) using HEDM to gain a comprehensive understanding of deformation mechanisms. By employing a high-energy X-ray beam and advanced data analysis techniques, we obtain detailed information about the crystallographic orientation, lattice elastic strain, and microstructure of Sn samples subjected to different loading conditions. The experimental data is analyzed using HEXRD, allowing us to reconstruct three-dimensional maps of the grain morphology, grain orientations, elastic strains, and corresponding stresses at the grain scale. Using HEDM analysis, we track the evolution of crystallographic defects in Sn during plastic deformation, providing crucial information for developing accurate constitutive models for performance predictions. This study demonstrates HEDM's potential for investigating the structural properties of materials, enabling improved understanding and control of their mechanical behavior.

Ashley Lenau

Program: Graduate Student
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Group: MST-8
Mentor: Reeju Pokharel
Discipline: Materials Science
Subject Area: Modeling and Simulation of Materials
LA-UR-23-27774

MODELING THE MICROSTRUCTURE EVOLUTION OF A 3D POLYCRYSTAL USING A RECURRENT NEURAL NETWORK WITH PHYSICS INFORMED LOSS FUNCTIONS

High energy x-ray diffraction is a state-of-the-art technique to study 3D microstructure evolution of materials and provides valuable information on how a single sample deforms. Crystal plasticity simulations using finite element or spectral methods may be faster than performing the experiment itself but are still computationally expensive to model evolutions of large 3D microstructures. Machine learning algorithms have faster generation times by several orders of magnitude but lack numerical accuracy compared to these numerical methods. In this research, a recurrent neural network is used to predict the microstructure evolution of a copper polycrystal at different strain increments. Given previous states of the microstructure, the network predicts the elastic strain and crystal orientation at the next strain step. The loss function incorporates fundamental equations describing the system, like Hooke's law, disorientation, and stress equilibrium, to enforce the physical boundary conditions of the system and increase the accuracy of the network predictions.

Gerson Leonel

Program: Graduate Student
School: Arizona State University

Group: EES-16
Mentor: Hongwu Xu
Discipline: Materials Science
Subject Area: Chemical Engineering
LA-UR-23-27942

SYSTEMATIC INVESTIGATION OF CO2 ADSORPTION ENERGETICS IN METAL ORGANIC FRAMEWORKS BASED ON IMIDAZOLYL LINKERS

This work explores systematics in the energetics of CO_2 adsorption in three 3-dimensional (3D) metal organic frameworks employing imidazolyl ligands, namely ditopic 2-methylimidazole (HMeIm) in $Zn(MeIm)_2$ (ZIF-8), $Co(MeIm)_2$ (ZIF-67), and tetratopic tetrakis(imidazolyl) boricacid ($HB(MeIm)_4$) in $CuB(MeIm)_4$ (Cu-BIF-3). All frameworks have the sodalite (SOD)topology. Direct gas adsorption calorimetric experiments enable quantitation of energetic drivefor CO_2 confinement in the frameworks. The general trend in the integral adsorption enthalpy ΔH_{int} (kJ/mol) is Cu-BIF-3 > ZIF-8 > ZIF-67. In Zeolitic imidazolate frameworks (ZIFs), greater porosity is consistent with more favorable CO_2 incorporation. Overall, the use of larger linker in boron imidazolate frameworks (BIFs) provides greatest enhancement of the energetics for CO_2 adsorption in Metal Organic Frameworks (MOFs). The strength of guest-host interactions depends on choice of metal and linker. Future work will investigate thermodynamic stability in uranyl and rare-earth MOFs.

Grant Martin

Program: Graduate Student
School: University of Oregon

Group: MST-7
Mentor: Cyndy Welch
Discipline: Materials Science
Subject Area: Polymer Science
LA-UR-23-27129

ENHANCING PLASTIC RECYCLING THROUGH NANO-SCALE STRUCTURE ANALYSIS IN CUSTOM BLOCK COPOLYMER FILAMENTS

Polymers provide outstanding mechanical properties while maintaining a lightweight and flexible physical profile. Block copolymers contain two or more immiscible polymer blocks that undergo self-assembly processes to form nano-scale structures. These unique crystal-like structures influence mechanical properties and compatibility with other plastics. This study uses small angle X-ray scattering (SAXS) to identify nano-scale structures inside custom-made block copolymer filaments. The filaments are used in a LulzBot Mini 2 FDM (fused deposition modeling) 3D printer to print complex shapes. The printed shapes will be tested to understand how the orientation of the nano-scale structure changes mechanical properties. This testing will be compared with a well-studied filament, ABS (acrylonitrile-butadiene-styrene), to quantify our results. Eventually, the custom filaments will be used in upcycling applications to improve plastic recycling.

Cassidy Mazelin

Program: Graduate Research Assistant
School: University of Oregon

Group: MST-7
Mentor: Ethan Walker
Discipline: Materials Science
Subject Area: Surface Engineering
LA-UR-23-27979

FABRICATION OF ANTI-CORROSIVE METAL OXIDE COATINGS ONTO STAINLESS STEEL BY CHEMICAL SOLUTION DEPOSITION

Metal oxide coating fabrication is commonly done by physical vapor deposition (PVD) and chemical vapor deposition (CVD). However, these methods prove challenging for industrial scale up. Chemical solution deposition (CSD) proves to be a cost-effective alternative that can be done by simply dipping or spraying a substrate to produce a film. Here various metal nitrate-hydrate coatings are explored for their abilities to decompose into thermally stable oxide compounds after annealing that exhibit non-wettability when coming into contact with molten metals. Zr, Er, Y, Nd, and Cr nitrates were tested by thermogravimetric analysis (TGA) to determine degradation profile for the proper annealing temperature. Sprayed and dipped stainless steel samples were also characterized via scanning electron microscopy and energy dispersive x-ray spectroscopy (SEM/EDS). Future characterization of the coatings includes focused ion beam (FIB), contact profilometry, molten contact angle measurement, and x-ray diffraction (XRD). Scale up of the CSD method has also been done using a custom tube furnace vacuum dip coater.

Charles Meyer

Program: Graduate Student
School: University of Texas at El Paso

Group: MST-16
Mentor: Meghan Gibbs
Discipline: Materials Science
Subject Area: Metallurgical and Materials Engineering

LA-UR-23-27633

CORRELATION OF INTERNAL MELT TEMPERATURE WITH EXTERNAL DIAGNOSTICS

Pyrometer readings can give useful information about the temperature of an object's surface. Pyrometer placement in induction casting experiments is important as this can dictate how similar the readings can be when comparing the outside of a crucible and a thermocouple within the melt. Depending on the placement, values can be as close as a 1°C or as far as 100°C. Several experiments were run with differing pyrometer readout placements. These experiments show that the closer the pyrometer readout position is to the radio-frequency field of the induction coils, the larger the temperature differential between the internal and external readings.

Caleb Minasian

Program: Graduate Student
School: Michigan Technological University

Group: J-2
Mentor: Joshem Gibson
Discipline: Materials Science
Subject Area: Metallurgy
LA-UR-23-27542

HSLA-100: IMPACTS ON IMPULSIVELY LOADED VESSELS

LANL is currently experiencing problems in consistently meeting low temperature toughness requirements in thick forgings for impulsively loaded vessels used for explosion testing. To explore potential underlying causes, the sensitivity of HSLA-100 to cooling rate was evaluated given that cooling rate varies throughout thick-section components, such as those used in LANL vessels. Varying cooling rates can impact what phases form in the components and resultantly affect the mechanical properties of the part. Blocks (10.5”x8”x2”) of HSLA-100 were heated to 800 C and subsequently cooled via three different cooling methods (furnace cooling, air cooling, and water cooling) to mimic relevant cooling rates within various sections of a thick-section part. It was concluded that HSLA-100 is sensitive to cooling rate because the difference in the formed microstructures throughout thick-section components and the impact these microstructures have on low-temperature toughness performance.

Geronimo Robles

Program: Graduate Student
School: University of Texas at San Antonio

Group: MST-8
Mentor: Joshua White
Discipline: Materials Science
Subject Area: Nuclear Fuel materials
LA-UR-23-27044

RESPONSE OF THE U3SI2+50WT%UB2 COMPOSITE ALLOYED WITH AL, AL2O3, Y, Y2O3 IN HIGH TEMPERATURE OXIDIZING ATMOSPHERES

The development of high density fuel (HDF) compounds has investigated composite, such as U3Si2/UN and U3Si2/UB2, to take advantage of their high uranium density and thermal conductivity. In the composite form, the energetic degradation mechanism of U3Si2 has been improved upon. However, the response to high temperature oxidizing atmospheres (i.e. steam) at 1200 degrees C continues to prevent deployment in advanced nuclear power reactors. Elemental additions such as Al and Y are incorporated with the intent to form a passivating oxide to inhibit oxygen diffusion into the fuel. Alternatively, oxides like Al2O3 and Y2O3 are explored to impart strength as well as corrosion resistance. Here, work previously detailed on the fabrication of the U3Si2 + 50wt% UB2 composite alloyed with Al, Y, Al2O3 and Y2O3 is expanded upon by measuring its oxidation performance. Measurements are conducted via thermogravimetric analysis under steam environment. Phase analysis is also presented via SEM, EDS, and XRD.

Kamaya Ronning

Program: Undergraduate Student
School: University of Washington

Group: MPA-CINT
Mentor: Jennifer Hollingsworth
Discipline: Materials Science
Subject Area: Nanotechnology
LA-UR-23-27965

USING DIP-PEN NANOLITHOGRAPHY TO OPTIMIZE PLACEMENT OF PHOTON EMITTERS IN NANOANTENNAE

Single-photon emitters that can emit in only one direction are particularly interesting for quantum communications technologies. To create such emitters, we use dip-pen nanolithography to couple a single emitter, e.g., an ultrastable "giant" quantum dot (gQD), with a designed nanoantenna. A useful antenna is one shaped like a bullseye, e.g., metallic bullseye (silver or gold) embedded in a dielectric material like a polymer or aluminum oxide. For the bullseye to cause highly directional photon emission, the emitter needs to be placed in the bullseye center. We have achieved placement success of ~15-20%, which is at least 20-fold better than random placement. Here, our goal is to improve precision and reproducibility of single-emitter placement and repeat success across other substrates and materials. Through optical analysis of photoluminescence of the placed gQDs and imaging by atomic-force microscopy, we can confirm our progress and provide single-emitters/antenna couples to collaborators around the world.

Jessica Stanfel

Program: Undergraduate Student
School: Colorado School of Mines

Group: MST-16
Mentor: Mathew Hayne
Discipline: Materials Science
Subject Area: Metallurgical and Materials Engineering
LA-UR-23-27638

CORRELATING COOLING RATE TO MICROSTRUCTURE IN AN ALSIFE ALLOY

An AlSiFe alloy (99.39 Al, 0.14 Si, 0.42 Fe) was cast in a copper wedge mold instrumented with four thermocouples, each measuring at a different height in the mold. A wedge mold was used in this project as it is possible to obtain various cooling rates in a single casting. The superheat was altered between experiments to observe a change in each measured cooling rate across castings. The purpose of altering cooling rates is to determine the effect this variable has on the microstructure and intermetallic formation via metallography. The changes in superheat were correlated to changes in the cooling rate and the cooling rate was related to microstructure.

John Stockdale

Program: Post-Bachelor's Student
School: Grand Valley State University

Group: C-CDE
Mentor: Andrea Labouriau
Discipline: Materials Science
Subject Area: Polymer Science
LA-UR-23-27407

ENGINEERING BORON-POLYMER COMPOSITES THROUGH MULTIPLE MANUFACTURING TECHNIQUES

Although 10B is favored to shield thermal neutrons due to its large (n, γ) cross-section, few polymer composites containing high boron concentrations exist. Thus, this study employed diverse manufacturing techniques (direct ink write, fused filament fabrication, compression molding, foaming) to fabricate polymer composites containing 30wt.% to 80wt.% boron. Siloxanes, poly(lactic acid), and acrylonitrile butadiene styrene acted as the polymer matrix. Polyethylene glycol and carbon nanofibers resolved issues with high boron concentrations such as clogging of printing nozzles and crumbling of compression composites. Boron concentration, as well as additive and fabrication type utilized affected thermomechanical properties. For instance, thermal conductivity of siloxane composites measured 0.15 W/mK to 1.01 W/mK with increasing boron concentration, whereas the maximum compressive strain was 78% at 0.6 MPa for the most porous foam.

Xavier Torres

Program: Post-Bachelor's Student
School: University of New Mexico

Group: C-CDE
Mentor: Andrea Labouriau
Discipline: Materials Science
Subject Area: Polymer Science
LA-UR-23-27776

INTERPLAY BETWEEN SHELF LIFE AND PRINTABILITY OF SILICA-FILLED SUSPENSIONS

Although fumed silica/siloxane suspensions are commonly employed in additive manufacturing technology, the interplay between shelf life, storage conditions, and printability has yet to be explored. In this work, Direct-Ink-Write (DIW) was used to print unique three-dimensional structures that required suspensions to retain shape and form while being printed onto a substrate. Suspensions containing varying concentrations of hydrophobic and hydrophilic silica were formulated and evaluated in terms of equilibrium storage modulus ($G'eq$) and yield stress (σy) for a time span of thirty days. Storage conditions included low and high relative humidity levels and temperatures ranging from 3°C to 25°C. This work aimed to establish the best storage conditions that will lead to longer shelf life and good printability of suspensions commonly used in DIW technology. These experiments showed a decrease in G' values and increases in G" over time as well as the printability decreasing overtime for our samples.

Mathematics

Facundo Airaudo

Program: Graduate Student
School: George Mason University

Group: CCS-2
Mentor: Aditya Pandare
Discipline: Mathematics
Subject Area: Numerical Methods Development
LA-UR-23-26903

DEVELOPMENT OF A HIGH-ORDER NUMERICAL METHOD FOR HYPER-ELASTICITY IN A MULTI-MATERIAL FORMULATION

An Eulerian formulation for the governing equations of solid mechanics of isotropic hyperelastic materials is presented. A high-order Discontinuous Galerkin (DG) finite element method is developed to discretize this system in space on unstructured 3D meshes. The method comprises the evolution of the deformation gradient tensor, and thermodynamically consistent closure models that relate internal energy to the stress tensor. Additionally, Riemann solvers depending on the physical acoustic speed in the solid material are used. This results in a novel approach, as very little research has been devoted to hyper-elastic problems using DG schemes or unstructured meshes. The above ideas are implemented in Quinoa- an open-source distributed-memory parallel 3D hydrodynamics solver with dynamic load balancing. The developed numerical method is verified using 1D and 3D benchmark problems.

Leah Howell

Program: Undergraduate Student
School: University of North Carolina at Chapel Hill

Group: CCS-7
Mentor: Andres Quan
Discipline: Mathematics
Subject Area: Applied Mathematics
LA-UR-23-27673

SYSLOG MESSAGE CLASSIFICATION USING MACHINE LEARNING

Darwin is an ASC funded, research testbed cluster. It is very heterogeneous, offering a wide variety of hardware, including x86, Power PC and ARM CPU architectures, systems with terabytes of memory, and a variety of GPUs and other accelerators. Darwin produces a stream of syslog messages which can be used to diagnose issues with particular nodes. Due to Darwin's design, messages from different nodes that might indicate the same issue can be written differently, complicating the diagnosis process. This project explores the efficacy of traditional machine learning models and large language models in classifying performance anomalies to combat this problem.

Svetlana Riabova

Program: Graduate Student
School: University at Buffalo

Group: T-5
Mentor: Hassan Hijazi
Discipline: Mathematics
Subject Area: Operations Research
LA-UR-23-22108

COORDINATED SPACE DOMAIN AWARENESS

Next generation systems for Space Domain Awareness will deploy networks of intelligent agents acting in the environment, requiring a mix of collaborative and individual behavior to accomplish their mission. Despite rapid progress on multiple fronts, effective coordination between agents remains one of the main barriers to wider adoption. Here we present a solution based on the idea of using a market-place model to represent interactions within distributed multi-agent sensor networks designed to coordinate activity of sensor ecosystems with diverse sensing capabilities, but limited resources, and no strict centralized control.

Abigail Schmid

Program: Graduate Student
School: University of Colorado Boulder

Group: XCP-8
Mentor: Stephen Andrews
Discipline: Mathematics
Subject Area: High Explosives, Bayesian Statistics
LA-UR-23-26802

BAYESIAN PARAMETER CALIBRATION FOR DAVIS REACTANTS EQUATION OF STATE

This study aims to identify optimal parameter values in the Davis Reactants Equation of State (EOS) for the high explosive (HE) PBX 9501. In pursuit of this goal, we solve the Bayesian inverse problem to identify parameter sets given experimental data. The experimental data include Hugoniot, specific heat capacity, and thermal expansion tests on the HE and its components. Previous calibrations have assumed 10\% error in the experimental data, but here we simultaneously estimate the unspecified experimental errors and EOS parameters. We estimate that the errors range between 5 - 30\%. We solve the Bayesian inverse problem with two methods, a Variational Bayesian approach and Markov Chain Monte Carlo (MCMC) algorithm, and compare the resulting parameters. We also analyze the covariance of the parameter estimates. This work identified parameters, with uncertainty, similar to previous calibrations of the EOS for PBX 9501 and adds information about the experimental errors.

Aleksei Sorokin

Program: Graduate Student
School: Illinois Institute of Technology

Group: T-6
Mentor: Nick Hengartner
Discipline: Mathematics
Subject Area: Probabilistic Numerics
LA-UR-23-28132

PROBABILISTIC MODELS FOR PDES WITH RANDOM COEFFICIENTS

PDEs with random coefficients often require expensive computations to produce inexact solutions. Functions of the solution process require solving for a large enough number of realizations that building a surrogate solution process proves valuable. This surrogate enables practitioners to quickly estimate functions of the solution process. We opt to efficiently fit a noisy Gaussian process surrogate and intelligently select the variance of the noise based on convergence of numerical solution errors. Specifically, we assume the error in truncating the dimension of the random coefficient and the error in discretizing the domain are independent. This enables us to refine the dimension and mesh width in an alternating fashion to approximate convergence rates and intelligently upper bound the Gaussian process noise error. We demonstrate our methodology on Darcy's equation for subsurface flow through porous media. Optimizations for fitting large scale Gaussian processes are also provided.

Other (Non-Technical)

Sydney Manginell

Program: Undergraduate Student
School: Northeastern University London

Ava Pietryga

Program: Undergraduate Student
School: University of Arizona

Sophia Mamula

Program: Undergraduate Student
School: University of New Mexico

Catarina Tchakerian

Program: Post-Master's Student
School: Northeastern University

Group: WRS-NSRCMS
Mentor: Laura McGuiness
Discipline: Other (Non-Technical)
Subject Area: History
LA-UR-26950

SERENDIPITOUS DISCOVERY IN ARCHIVAL SPACES

Over the past several decades, archivists and researchers have witnessed the rapid expansion of digital archival collections. With this expansion comes the fear that opportunities for Serendipitous Information Encountering - the accidental discovery of useful or interesting information not originally sought after - are decreasing. Serendipitous discoveries are traditionally associated with browsing physical collections. Given the proven value of serendipity to research and innovation, memory institutions like the NSRC must address the challenge to replicate this experience within closed stacks and digital collections. By exploring factors that foster or inhibit accidental discoveries, we hope to suggest how the NSRC can create an environment that facilitates Serendipitous Information Encountering.

Jonathan Rascon

Program: Undergraduate Student
School: New Mexico Institute of Mining and Technology

Group: AOT-RFE
Mentor: Lawrence Castellano
Discipline: Other (Non-Technical)
Subject Area: Radio Frequency
LA-UR-23-27262

ASSEMBLY, WIRING, PROGRAMMING, AND DOCUMENTATION OF THE DLTC

The Los Alamos Neutron Science Center (LANSCE) 800-million-electron-volt (MeV) accelerator modernization project has been ongoing. One of the upgrades includes the RF transmission, Drive Line Temperature Control (DLTC) system. The main purpose (DLTC) chassis is to control a set temperature throughout the 201.25 MHz and 805 MHz reference lines. The 201.25 MHz is 295 feet long and the 805MHz reference line is 2,550 feet long. The DLTC Chassis was upgraded back in 2018, adding an OMEGA temperature Controller with Proportional, Integral, Derivative (PID) which is a closed loop temperature controller system, that has a with real time temperature read back communication and a monitoring system to control temperature of the transmissions line. The project is to assemble the mechanical chassis, then the electrical wire; updating both mechanical and electrical drawing if needed. The main purpose of this project is for future use and set all OMEGA Temperature Controller parameters.

Adriana Sanchez

Program: Post-Bachelor's Student
School: St. Olaf College

Group: WRS-NSRCMS
Mentor: Nicholas Lewis
Discipline: Other (Non-Technical)
Subject Area: Knowledge Capture and Preservation
LA-UR-23-28138

KNOWLEDGE CAPTURE AT LANL: LESSONS FROM ETHNOGRAPHY

Historically, emergency knowledge capture has been used as a way to collect information regarding a cultural environment. Originally artifact focused, ethnographers used "technology" from different cultures to help explain how a culture functions. Over time, knowledge capture has evolved into a more collaborative effort, featuring contributions from both the ethnographer (cultural information collector), and the interlocutor (cultural informant). LANL currently faces rapid knowledge loss as employees change positions within the institution, terminate lab employment, and retire. Current knowledge loss mitigation methods include artifact collection/preservation, interviews, and knowledge sharing events. While this methodology is helpful, there are additional ethnographic methodologies that can strengthen explanations of the "technique" aspects of culture, or how "technology" is learned and used. By introducing a more ethnographically based qualitative approach that incorporates the collection of tacit knowledge into knowledge capture, LANL has the possibility to expand upon the type of knowledge being captured.

Physics

Svetlana Backhaus

Program: High School Student
School: Calvert Academy

Group: P-4
Mentor: Heather Johns
Discipline: Physics
Subject Area: Thermonuclear Plasma Physics and Data Science
LA-UR-23-27475

ANALYZING TRENDS BETWEEN INITIAL CONDITIONS AND RADIATION AND SHOCK FRONT PROPAGATION IN COAX-INSPIRED RADFLOW EXPERIMENTS

Data analysis methods are used to develop a relationship between the initial conditions (laser drive energy and foam density) of the COAX and Radishock experiments and the propagation of an X-ray radiation wave and a hydrodynamic shock wave through a physics target. The goal is to develop an understanding of how laser energy and the density of a target influence the velocities of X-ray radiation and hydrodynamic shock waves through semi-homogeneous media. Another avenue of investigation is finding the influence of an X-ray radiation wave on the resulting shock wave and vice versa. Linear Regression models are generated using the Python module Statsmodels, then tuned and selected according to common Data Science practices. Finally, the assumptions of Linear Regression are checked within the best and worst performing models in order to address if another category of model is necessary to describe this complex relationship.

Luis Bichon

Program: Graduate Student
School: Vanderbilt University

Group: P-3
Mentor: Cesar Da Silva
Discipline: Physics
Subject Area: High Energy Nuclear Physics
LA-UR-23-28338

ELLIPTIC FLOW MEASUREMENT OF J/_ IN PHENIX RUN14 AU+AU AT √ SNN = 200 GEV

The Quark Gluon Plasma (QGP) produced in relativistic heavy ion collisions exhibits a nearly perfect fluid behavior. This behavior is observed as strong azimuthal correlations between the produced particles, but presently, the detailed interactions of the heavy quarks in the QGP medium are under investigation. The PHENIX experiment at RHIC has a unique coverage at forward rapidity and a large sample of J/ψ to dimuon decays collected in 2014 in Au+Au collisions at 200 GeV. At such an energy, in central collisions, this area of phase space yields the smallest fraction of $c\bar{c}$ pairs when compared to midrapidity, where most pairs are produced. With such yields, charmonium coalescence a dominating source of J/ψ elliptic flow (v2) may not be present. We present the first statistically improved measurement of J/ψ elliptic flow at RHIC energies at forward rapidity.

Timothy Coffman

Program: Post-Bachelor's Student
School: Texas A&M University

Group: P4
Mentor: Yongho Kim
Discipline: Physics
Subject Area: Plasma Physics
LA-UR-23-27719

INERTIALLY CONFINED FUSION EXPERIMENTS USING A 3D PRINTED SPHERICAL CAPSULE

Los Alamos National Laboratory's Bosque experimental platform investigates the effects of heterogeneous mix on thermonuclear burn, as well as explores the capabilities of 3D printed capsules. This experimental campaign on the OMEGA Laser Facility used 3D printed 2PP (two photon polymerization) plastic lattices inside spherical capsule shells that are filled with either H2 gas for carbon-deuterium-oxygen (CDO) printed lattices or D2 gas for carbon-hydrogen-oxygen (CHO) printed lattices. Experimental results were compared to numerical simulations, which assumes complete atomic mixing. Observed yields agree with the simulations in the case of the CHO lattices with a D2 fill gas; however, in the case of CDO lattices with an H2 fill gas the experiment produced lower yields than what the simulations predicted. This discrepancy is possibly due to the inadequacy of the assumption of thermal equilibrium between CDO lattices and H2 gas. This possible inadequacy of thermal equilibrium is further investigated through the analysis of Spectrally Resolved Electron Temperature (SRTe) diagnostics on the OMEGA platform. From this experimental campaign, predictive capabilities on the effects of material mix have been improved for on-going Bosque experiments on the National Ignition Facility.

Robert Dwyer

Program: Graduate Student
School: University of Rochester

Group: P-4
Mentor: Kevin Meaney
Discipline: Physics
Subject Area: Mechanical Engineering
LA-UR-23-28188

OPTIMIZATION OF THE GAMMA REACTION HISTORY DIAGNOSTIC FOR DOUBLE-SHELL CAMPAIGNS ON THE NATIONAL IGNITION FACILITY

Efforts are underway to understand the dynamics of volume burn and ignition in a laboratory environment by measuring gamma emission from D-T implosions on the double-shell platform by utilizing the Gamma Reaction History (GRH) diagnostic. The double-shell platform utilizes a high-Z pusher in direct contact with the fusion fuel and an outer low-Z ablator compared to the low-Z pusher on the NIF. The D-T nuclear reaction history curve provides critical information about the energy balance and loss mechanisms during thermonuclear burn. Information about the high-Z pushers used in volume burn platforms from (n,n') gamma production from inelastic scattering such as the time-resolved areal density of the pusher which yields energy transfer from the ablator to the pusher and pusher velocity. These measurements may help inform capsule design and constrain hydrodynamic codes. An optimization study of the GRH diagnostic to measure the D-T gammas and the (n,n') gammas from the high-Z pusher was conducted in anticipation of FY24 D-T double-shell implosions on NIF.

Francesca Elverson

Program: Post-Master's Student
School: University of Edinburgh

Group: C-PCS
Mentor: Pamela Bowlan
Discipline: Physics
Subject Area: Ultrafast Spectroscopy

LA-UR-23-28224

AUTOMATIC DIFFERENTIATION FOR PHASE RETRIEVAL TO MEASURE EXTREME ULTRAVIOLET FREE ELECTRON LASER PULSES

Free Electron Lasers (FELs) produce bright coherent ultrashort pulses in the extreme ultraviolet (XUV) to hard X-ray photon energy range, giving access to the fundamental spatial and temporal scales of matter. Essential for using FELs is the ability to characterize the pulse's electric field, E(t) e.g. to facilitate pulse shape optimization and interpretation of experimental data. Measuring such pulses is challenging, particularly due to their high photon energies. We build upon our recent work whereby a pulse characterization method called Frequency Resolved Optical Gating (FROG) was successfully adapted to measure XUV FEL pulses: involving the interaction of XUV and optical light pulses in a non-linear material outputting a spectrogram, from which a phase-retrieval algorithm can obtain E(t). We improve the phase-retrieval algorithm portion of the FROG technique by introducing autodifferentiation to improve the speed, accuracy, and modelling of the non-linear material response at high energies and use the new algorithm on experimental data taken at the FERMI FEL.

Ethan Fisk

Program: Undergraduate Student
School: Rensselaer Polytechnic Institute

Group: XTD-IDA
Mentor: Jarrett Johnson
Discipline: Physics
Subject Area: Astrophysics
LA-UR-23-28282

AN ASSESSMENT OF THE EFFECT OF ACTIVE GALACTIC NUCLEI ON THE MASS OF POPULATION III STAR CLUSTERS

Possible signatures of a Population III Star cluster have recently been discovered by the James Webb Space Telescope (JWST) in the vicinity of an Active Galactic Nucleus (AGN) (Maiolino et al. 2023). Simulations in the Enzo cosmology code were conducted to assess whether an AGN, modeled as an X-Ray background along with a Lyman-Werner (LW) background representing a stellar population within its own halo, could delay Population III star formation until a lower redshift wherein its dark matter halo could grow to a larger mass in order to host a larger cluster of stars. A cosmological simulation was run with a radiation field equivalent to an AGN ~20 kpc away.

William Gammel

Program: Graduate Student
School: University of Arizona

Group: XCP-6
Mentor: Joshua Sauppe
Discipline: Physics
Subject Area: Plasma Physics/Machine Learning
LA-UR-23-27332

OPTIMIZING CYLINDRICAL TARGET DESIGNS THROUGH GAUSSIAN PROCESS BASED SURROGATE MODELING

Reducing performance degradation factors, such as hydrodynamic instabilities, is crucial to inertial confinement fusion research. Cylindrical targets have shown promise in diagnosing instabilities while enabling direct diagnostic access. However, designing these experiments relies on complex 1D and 2D radiation-hydrodynamics simulations, which both hinders data collection and causes the optimization of such targets to be prohibitively expensive. To address this, we propose leveraging surrogate models based on Gaussian Processes (GPs) to significantly reduce optimization costs. The predictive capability of the surrogate model is first assessed, comparing it to other proposed machine learning techniques. Furthermore, we introduce an optimization algorithm rooted in Efficient Global Optimization (EGO) that utilizes the GP surrogate to discover cylindrical target designs that maximize yield while minimizing computational expense.The optimized design selected by EGO is discussed, highlighting both the design choices and implosion physics we believe to be responsible for the target's enhanced performance.

Abigail Hartley

Program: Undergraduate Student
School: University of Colorado Boulder

Group: CCS-2
Mentor: Irina Sagert
Discipline: Physics
Subject Area: Computational Physics and Methods

LA-UR-23-26763

SIMULATING BINARY NEUTRON STAR MERGERS WITH SOLID CORES

Neutron stars are among the densest objects in the Universe, yet the nature of their cores remains a mystery. Many alternatives were suggested, involving exotic particles and new states of matter, such as hyperons, deconfined quark matter, etc. One of the intriguing possibilities is a crystallized solid quark matter. Our project aims to test this hypothesis by computing gravitational wave signals from mergers of stars with solid quark cores, and comparing them to the GW signatures from mergers of stars with fluid cores. We use the LANL Smoothed Particle Hydrodynamics (SPH) code, FleCSPH, to simulate binary neutron star mergers with solid quark matter cores. FleCSPH describes the dynamics of terrestrial and astrophysical solids, allowing us to accurately assess the effects of various solid cores on GW signals from neutron star mergers. We conduct parameter studies of binary mergers using different parameters of our strength model and nuclear equations of state.

Eibhleann Hinrichs

Program: High School Student
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Group: P-1
Mentor: Andrea Albert
Discipline: Physics
Subject Area: Astrophysics/Particle Physics
LA-UR-23-27692

SEARCHING FOR DARK MATTER WITH HAWC

Dark matter is a mysterious astronomical substance with the gravitational ability to hold galaxies together. What exactly dark matter is, we cannot say for certain. However, it is plausible that some sort of axion-like particle could be responsible for the presence of this gravitational substance in outer space. Axion-like particles, or ALPs, are hypothetical particles that interact very rarely, if at all. Using the High-Altitude Water Cherenkov gamma ray observatory, we are setting upper limits to possible ALP models. ALPs also have very high energy signatures; thus, we can use the latest and greatest HAWC dataset to study them. So far, we do not see signals and so can rule out models of ALPs that would have given a signal. These are known as upper-limits, and once they are determined, this information is sent to collaborators in Stockholm led by Sunniva Jacobsen for analysis with regards to particular ALP models.

Alexander Holas

Program: Graduate Student
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Landon Dyken

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Program: Graduate Student
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Mark Ivan Ugalino

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LA-UR-23-27015

ARES - A PERFORMANCE PORTABLE TOOL TO SIMULATE SUPERNOVAE BASED ON THE PARTHENON FRAMEWORK

Historically, codes for simulating supernovae (such as Arepo, FLASH or LEAFS) have been at the forefront of scientific high-performance computing due to the immense computational resources required for full 3D simulations. However, given the shift towards heterogeneous HPC architectures, many current-generation codes are at the risk of losing their competitiveness as they are only designed to run on homogeneous CPU-only systems. There exist several efforts to enable these codes for GPU's, however, these efforts only consider specific architectures or vendors (e.g., implement only CUDA or HIP), limiting themselves to a small range of exascale computing systems. Frameworks such as Kokkos aim to provide an environment which is agnostic of the targeted architecture, enabling the development of performant and portable code. In the Ares code, we develop a performance portable tool to simulate supernovae based on the Parthenon Framework, which in turn uses Kokkos in the background. Here, the Parthenon Framework provides an interface to the underlying mesh-refinement routines, which form the backbone of our code. In addition, we incorporate the already existing Singularity-EOS toolkit to provide us with various equations of state, primarily the Helmholtz equation of state. We also include the JINA Reaclib as a basis for our nuclear network solver. Finally, we implement a gravity solver to complete the required physics. We verify the proper operation of the Ares code with various established initial conditions such as a Rayleigh-Taylor instability and a shock tube. Lastly, using this minimal codebase, we simulate a centrally ignited detonation of a carbon-oxygen white dwarf, verifying its capabilities as a supernova code the results against simulations of tried-and-tested codes such as Arepo. We use this setup to explore the scaling of the Ares code on various architectures in order to establish that our code can form the basis for a futureproof and performance portable supernova code.

Madison Howard

Program: Graduate Student
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Group: J-6
Mentor: Joshua Coleman
Discipline: Physics
Subject Area: Accelerator Physics
LA-UR-23-27629

EVALUATING EMISSION CHARACTERISTICS OF VELVET CATHODES ON MICROSECOND TIMESCALES

Velvet is a common material utilized for electron emission and is used in the Axis-I injector at the Dual Axis Radiographic Hydrodynamic Testing Facility (DARHT) at LANL. Velvet emitters are not well documented or diagnosed on microsecond timescales. This is due to a high expansion velocity, which makes it unideal for accelerator applications. The Cathode Test Stand (CTS) is designed to test velvet cathodes over long pulse durations, along with various other field emitters and photocathodes. Various diagnostics are employed on the CTS to measure extracted beam current, current density, and electron and x-ray scatter. This presentation will highlight these measurements as well as document the lifetime of a velvet sample.

Patrick Lohr

Program: Graduate Student
School: University of Arizona

John Cappelletti

Program: Graduate Student
School: University of Rochester

Group: XCP-DO
Mentor: Finkelstein, Josh
Discipline: Physics
Subject Area: Computational Physics
LA-UR-23-27513

ACCELERATION OF ORBITAL-FREE DENSITY FUNCTIONAL THEORY USING DISTRIBUTED FAST FOURIER TRANSFORMS ON GPUS

Orbital-free density functional theory (OF-DFT) is a first-principles computational method that is commonly used to study the electronic structure of many-body systems in the warm dense matter (WDM) regime. Unlike Kohn-Sham DFT, which becomes cumbersome in the WDM regime due O(T3N3) scaling, OF-DFT scales linearly with system size due to implicit dependence on the total electron density, increasing the computational efficiency of large high-temperature calculations by many orders of magnitude. The OF-DFT code, Stochastic and Hybrid Representation Electronic structure by Density functional theory (SHRED), developed at LANL, utilizes fast Fourier transforms (FFTs) and the conjugate gradient (CG) method of minimization to perform ab-initio molecular dynamics using the Fermi-Dirac-von Weizsäcker model. By offloading the execution of these algorithms to GPUs, significant improvements to computational efficiency can be gained. Our results indicate that NVIDIA's cuFFTMp library has the potential to rapidly accelerate the performance of SHRED on Chicoma.

Michael Martin

Program: Undergraduate Student
School: Michigan Technological University

Group: ISR-1
Mentor: Kelly Malone
Discipline: Physics
Subject Area: High Energy Astrophysics
LA-UR-23-27523

CREATING AN HIGH ENERGY ALERT SYSTEM FOR THE HAWC GAMMA RAY OBSERVATORY

One of the greatest mysteries in astrophysics is exactly how Cosmic Rays (CRs) are accelerated up to extremely high energies within our galaxy. Hadronic models of possible CR accelerators, including supernova remnants and pulsars, require the production of both gamma rays and neutrinos at these sources. Searching for coincidences between neutrino and the highest energy gamma ray observations can help confirm these theories. The High Altitude Water Cherenkov (HAWC) observatory is a ground based gamma ray observatory located at 4100m in Puebla, Mexico. HAWC is able to detect gamma rays with energies greater than 100 TeV, has a wide field of view, and a 95% duty cycle, making it ideal for these types of coincidence searches. This work aims to create a high energy alert system for HAWC, sending out an alert to other experiments for gamma ray events it sees above 56 TeV.

Phillip Martin

Program: Post-Bachelor’s Student
School: Cornell University

Group: MPA-Q
Mentor: Katarzyna Krzyzanowska
Discipline: Physics
Subject Area: Quantum Information Science
LA-UR-23-27693

METROLOGY BEYOND THE SQL WITH MIXED STATES AND BEC

Atom interferometers exploit the wave nature of ultracold atoms for measuring acceleration, rotation, gravity, and electromagnetic fields. The performance of a typical atom interferometer is limited by two factors: the coherence time of the system, and the Standard Quantum Limit (SQL). While the coherence time typically depends on the experimental implementation, the SQL is a fundamental limit that comes from a projection noise of measurements. The improvement of the device’s performance can be achieved by introducing quantum correlations that enable phase measurement below the SQL, reaching the Heisenberg limit for a fully entangled system. We numerically study a metrology protocol that utilizes an ancilla qubit (a single atom) interacting with an ensemble of qubits (atoms in Bose Einstein condensate–BEC) under imperfect experimental conditions. The expected noise channels include imperfect entangling gate fidelity, statistical fluctuation of atom number N, and leakage of information due to loss of atoms.

David Nystrom

Program: Undergraduate Student
School: University of Arkansas

Group: P-4
Mentor: Eric Loomis
Discipline: Physics
Subject Area: Computational Physics
LA-UR-23-27775

MULTI-SHOCK DESIGN TOOLS IN DOUBLE SHELL MODELS

In this project, current proposed models describing the “Radiation Temperature”-”Laser Power” relationship within a Hohlraum are analyzed through Python emulation and hydrodynamics simulation. Primary objectives were to confirm the validity of an approach laid out in D. Callahan’s paper1, while also adapting it to the double shell case. This led to the production of user-friendly code assisting in navigating the data. ICF researchers benefit by gaining immediate insight into indirect double-shell target physics.

Henry Prager

Program: Graduate Student
School: New Mexico Institute of Mining and Technology

Group: XTD-IDA
Mentor: Joyce Guzik
Discipline: Physics
Subject Area: Astrophysics
LA-UR-23-27845

A PARAMETER STUDY OF 1D ATMOSPHERIC MODELS OF PULSATING AGB STARS

Asymptotic Giant Branch stars are roughly solar mass stars that are in the final stages of stellar evolution, losing their stellar envelopes and becoming white dwarfs. The mass-loss process occurs through a complex interaction of the stellar atmosphere being levitated and shocked by pulsations and entertainment of the levitated gaseous atmosphere with the dust produced there [1, 2, 3, 7]. Models have greatly informed our understanding of this process, but the numerical details of the process are still weakly determined. In this study, we have run several grids of atmospheric models of AGB stars. With these grids, we can quantify the effects of adjusting individual model parameters. In addition, we can compare how atmospheric models grids with typically assumed values compare to observation, and with the results of the parameter study determine the model parameters needed to bring models into agreement with observations.

Marvyn Raya

Program: Undergraduate Student
School: Rice University

Group: AOT-AE
Mentor: Haoran Xu
Discipline: Physics
Subject Area: Accelerator Physics
LA-UR-23-27606

CERAMIC ENHANCED ACCELERATOR STRUCTURES

Accelerating structures use metallic resonant cavities to accelerate electron beams. By utilizing a ceramic insert within an accelerator structure power is saved. We see this increase in efficiency because ceramics are insulators, thus the ohmic loss does not happen inside the ceramic insertion. As a result, the unique ceramic enhanced accelerator structure (CEAS) design produces a high shunt impedance. This means the accelerator can more efficiently convert supplied radio-frequency (RF) power to accelerating gradient. Such an efficient structure allows us to use particle accelerators in extreme conditions. For instance, the CEAS can be used in space to produce electron beams that generate plasma waves by interacting with space plasma.

Jacob Roybal

Program: Undergraduate Student
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Group: AOT-AE
Mentor: Huang En-Chaun
Discipline: Physics
Subject Area: Particle Accelerator Physics
In Process

BEAM MEASUREMENTS WITH PSR

The project I have been working on includes the usage of an oscilloscope and that is controlled remotely by using both Python and the SCPI. With these tools I was able to take different measurements and capture different wavelength forms. The PSR could serve as a sensitive mass spectrometer once protons circulate the ring for many turns due to its precise circumference and well-measured magnetic fields. In this project we demonstrate the comparison of beam energy measurements via monitor signals and reference frequency.

John Schmidt

Program: Post-Bachelor's Student
School: Iowa State University

Group: P-1
Mentor: William Meijer
Discipline: Physics
Subject Area: Accelerator Physics
LA-UR-23-27540

UNIQUE MAGNET MAPPING SYSTEMS FOR BEAM OPTICS DEVELOPMENT

The development of new magnetic optics requires well known magnetic field maps. This was the motivation behind creating new quick and reliable magnet mapping systems. The main system is a rotating hall probe set up that is able to reliably measure the excitation curve, fringe (Enge) coefficients, and multipole components. In this poster I will go over the design, the data and analysis, as well as the motivation for a new magnet mapping system.

Ryan Scott

Program: Post-Bachelor's Student
School: Brigham Young University

Group: XTD-IDA
Mentor: Mike Tamashiro
Discipline: Physics
Subject Area: Nuclear Physics
LA-UR-23-27781

EXPLORATION OF DOUBLE SHELL INERTIAL CONFINEMENT FUSION CAPSULE DESIGN PARAMETERS AND YIELD

The Common Modeling Framework (CMF) is a suite of tools to help users create simulations to run on high-performance computers. Developing and using these tools, I have created a parameter study of double shell inertial confinement fusion (ICF) capsules which will be simulated using xRage. This parameter study includes fill tubes that will be used in actual experiments next year as well as more ideal fill tubes to help characterize how capsule energy output (yield) varies with fill tube size.

Enrique Segura Carrillo

Program: Guest Student
School: University of Colorado Boulder

Group: MPA-Q
Mentor: Michael Martin
Discipline: Physics
Subject Area: Quantum Information Science
LA-UR-23-27940

CHARACTERIZING ENERGY SPECTRUM OF BLUE-DETUNED OPTICAL BOTTLE BEAMS FOR COLD RYDBERG ATOM TECHNOLOGIES

Ultracold Rydberg atoms are promising building blocks for large, scalable, robust quantum architectures. Blue-detuned optical Bottle Beams (BoBs) create a tightly confining 3D optical potential in which cold atoms will be trapped and localized. By imprinting a phase mask on an incoming beam with a spatial light modulator, a dark focus surrounded by light suitable for atom trapping is created. BoBs possess attractive features for atom storage: reduced atomic heating, photon scattering, light shifts, and decoherence rates, thereby enhancing atomic lifetimes. Trapping at an intensity minimum enables simultaneous control of both ground and Rydberg states, making BoBs ideal for coherent quantum control. Furthermore, its optical potential is harmonic in its axial direction z, and quartic in its radial direction. The anharmonicity in BoBs enables a host of quantum engineering applications. We investigate atom trapping of Rubidium and Strontium using BoBs and estimate their corresponding energy spectra.

Marian Stradling

Program: Undergraduate Student
School: Brigham Young University

Group: XTD-IDA
Mentor: Jarrett Johnson
Discipline: Physics
Subject Area: Astrophysics

LA-UR-23-27476

ACCRETION DISK RADIATION AND HOW IT AFFECTS THE GROWTH OF A SUPERMASSIVE BLACK HOLE

As gas falls into a supermassive black hole, a fraction of the gas' mass is radiated back as photon energy. That same energy disrupts other gas falling into the black hole and pushes particles away from the black hole, which lowers the rate at which the black hole accretes. Different photon energies disrupt the gas at different magnitudes, which changes the accretion rate of the black hole. Using the cosmology code Enzo, we ran several simulations of a black hole with an initial seed mass of one million solar masses at a redshift of twenty. For each simulation, we set the black hole to only release a specific photon energy (ie. 2eV, 14eV, 5190eV). Using the simulations, we compared the total masses and accretion rates at a redshift of six.

Nathan Ward

Program: Undergraduate Student
School: University of Southern California

Group: MPA-Q
Mentor: Raymond Newell
Discipline: Physics
Subject Area: Quantum Physics
LA-UR-23-27939

CAVITY STABILIZATION IN THE GENERATION OF SQUEEZED LIGHT

A source of squeezed light is a fundamental building block for photonic quantum computing. In squeezed quantum states, noise in one quadrature is “squeezed” below the standard quantum limit. Squeezed light is typically produced in an optical cavity with a nonlinear crystal. The wavelength of the laser driving the cavity must be well matched to the cavity length, and temperature control of the nonlinear crystal is essential. In this work, we employ the Pound-Drever-Hall (PDH) technique to control cavity length. In the PDH technique, the length of the cavity is controlled to maximize coupling into the cavity. A custom heating plate consisting of a copper stand heated by a Peltier element maintains constant temperature of the crystal. Both applications rely on a feedback loop using the proportional, integral, derivative (PID) control algorithm to control their respective process variables.

Samuel Wescott

Program: Undergraduate Student
School: University of Arizona

Group: AOT-AE
Mentor: Charles Taylor
Discipline: Physics
Subject Area: Particle Accelerators
LA-UR-23-28444

DETERMINING LANSCE LINAC ENERGY SPREAD VIA ARCHIVED WIRE-SCANNER DATA

When redirecting the LANSCE H - beam to the attached research facilities, variations in the particles' energy when passing through a magnetic field result in a horizontal spread observable using wire-scanners. A change in the beam size would potentially increase beam losses in the high energy beam transport region and in the proton storage ring (PSR). Higher beam losses is often one of the major limitations for LANSCE to achieve higher current for the user facilities. Over the past several years, data has been collected regarding this; however, minimal analysis has been done. This project uses Python to fit Gaussian curves to the data, for easier comparison. Using the aggregated plots, various metrics can be compared to search for any noteworthy change over time in the performance of the accelerator, focusing primarily on the standard deviation.

Jackson White

Program: Graduate Student
School: University of Texas at Austin

Group: XCP-5
Mentor: Charlie Starrett
Discipline: Physics
Subject Area: Plasma Physics
LA-UR-23-27818

PSEUDOATOM MOLECULAR DYNAMICS PLASMA MICROFIELDS

Stark broadened line shape profiles are crucial for diagnosing hot dense plasma spectra, including both laboratory experiments and astrophysical observations, because they model the broadening of observed bound-bound atomic transitions. A key input to analytic line shape models is the plasma microfield, which is the expected distribution of low-frequency E-fields generated by a plasma. We present a new method of calculating plasma microfields using the pseudoatom molecular dynamics (PAMD) code. We have implemented the capability to model an atomic species with an arbitrary bound electron configuration in a pseudoatom plasma, enabling the calculation of microfields for different charge states and different electron configurations within the same plasma. In this poster we present initial results from this new method of calculating the microfield and highlight PAMD's treatment of ion-electron correlations.

Parker Willis

Program: Undergraduate Student
School: Rice University

Group: XTD-NTA
Mentor: Jarrett Johnson
Discipline: Physics
Subject Area: Computational Astrophysics

LA-UR-23-27796

IMPACT OF BLACK HOLE SEED MASS ON QUASAR ACCRETION

Quasars are some of the brightest objects in our universe, and we know little about how they form and grow. With the James Webb Space Telescope (JWST), we have discovered quasars that are extremely massive early in our universe, giving us clues as to how they form. Using the cosmological simulator Enzo, we attempted to simulate black holes (BHs) with different initial masses to see if we can recreate the conditions needed to form a quasar like those seen with JWST. We started by seeding a BH at z = 20 with initial masses between 100,000 and 10,000 $M_\odot$ in a dark matter halo with a mass of 4 x 107 $M_\odot$. We used a flux accretion prescription with radiative transfer feedback. We recorded the change of the BH's mass and the accretion rate over time. We related our finding to some of the quasars newly discovered by JWST.

Thank you for participating!

-The Student Programs Office-

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