

# 19TH ANNUAL 2019 STUDENT SYMPOSIUM PROJECT ABSTRACTS

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# **BIOSCIENCES**

**Amber Abbott**

Program: UGS/Postbac

School: Virginia Tech

Group: B-10

Mentor: Shawn Starckenburg

Category: Biosciences

Type: Individual

LA-UR: 19-25521

**Environmental conditions causing mating of green alga Scenedesmus**

Selective breeding of agricultural plants is ancient and universal, allowing for increased crop yield, resistance to predators and pests, and tolerance of environmental pressures. However, it is not yet possible to selectively breed industrially relevant species of algae, despite their growing potential for use as a food and fuel source. It has recently been established that it is possible to induce sexual reproduction in some algal species under certain conditions, which would provide a means for selective breeding. One such species is the eukaryotic green algae *Scenedesmus obliquus*. Water samples will be collected from the Los Alamos Reservoir and the algal cells cultured for a week, then *S. obliquus* will be identified and isolated through sequencing techniques and visual confirmation. Sexual reproduction of the cultures will be induced through nitrogen deprivation and cold temperature shock, and confirmed by observing elongated cell shape, flagellation, and increased motility. From the results, mating protocols will be developed by varying these conditions systematically in order to enable future breeding practices.

## **Dara Armstrong**

Program: High School

School: Los Alamos High School

Group: T-6

Mentor: Christopher Neale

Category: Biosciences

Type: Individual

LA-UR: 19-26792

## **Studying Ras Deactivation Through Molecular Dynamics Simulations**

Ras, a protein that regulates cell growth, is a driver behind many different types of cancer. Ras regulates cell growth by acting as an on-off switch; when the switch is on, cells grow and divide, and when the switch is off, cells do not grow or divide. Certain mutations occurring in the Ras protein, cause the switch to be on for extended amounts of time and cause Ras to constantly be in its activated state. This triggers uncontrolled cell growth, and can lead to cancerous tumors. Thus, a critical part of normal cell growth regulation is the deactivation of Ras. By understanding the mechanisms behind how Ras deactivates, critical information will be unlocked and we may be one step closer to the possibility of creating drugs that help deactivate Ras. One main goal of molecular dynamics simulations is to create data that agrees with experimental data. However, in the simulations we created, Ras deactivates much faster than experimental data suggests it should. To figure out why this is the case, we are using the protein database (PDB) to find as many other structures of active Ras protein as possible and then using these structures as input for molecular dynamics simulations. By observing many different Ras proteins in simulations and noting similarities and differences among them, we will gain important information about the nature of Ras deactivation, and hope to use this information to improve our model for the study of Ras deactivation.

## **Keisha Avery**

Program: GRA/Post Masters  
School: University of Missouri - Columbia  
Group: B-11  
Mentor: John Dunbar

Category: Biosciences  
Type: Individual  
LA-UR: 19-26459

### **Factors affecting species migration into preexisting microbial communities: a meta-analysis**

Inoculation of microbial species into preexisting microbial communities is a strategy to improve the function of microbial communities and the systems they inhabit (e.g. human guts,...). There are many factors that may influence the success of establishment of inoculated microbes in preexisting communities. Possible factors include characteristics of the target environment, characteristics of the inoculant, and how the inoculant is delivered. However, it is unknown which factors contribute the most to establishment. To address this knowledge gap, we are performing a meta-analysis of published studies that examined factors influencing the success of species migration into preexisting microbial communities and the associated effects on community or ecosystem function. Understanding the factors that facilitate successful species migration is a foundation for applications in human, animal, plant, and soil health.

## **Ryan Bermel**

Program: UGS/Postbac

School: New Mexico State University

Group: B-11

Mentor: Ramesh Jha

Category: Biosciences

Type: Individual

LA-UR: 19-26438

### **Renewable plastic production using engineered microbes**

Plastic has become one of the most ubiquitous and indispensable materials used in every area of society; from the food industry for packaging, to construction, household goods, and even to high grade scientific equipment. The world economy relies heavily on the inexpensive production of plastic. An estimated 300 M tons of plastic were produced in year 2014, and the number is expected to go up more than 3-fold to 1.1 B tons by the year 2050. However, at this time almost all industrial production of plastic stems from petroleum-derived chemicals resulting in release of high amount of greenhouse gases in the environment, as well as being produced from a finite resource. Therefore, to be able to develop a sustainable economy, a renewable source of plastics must be developed. In this respect, we are engineering microbes, which are capable of using simple sugars and converting them into Terephthalate (TPA, a constituent of ubiquitous PET plastics). Benzoate can be renewably produced from sugars, and a para- carboxylation of this molecule will form TPA. Some microbes have naturally evolved enzymes to decarboxylate certain carboxylic phenols (4-hydroxybenzoate phenol) to use as a carbon source for growth. Such enzymes can also perform reverse reactions (for example phenol 4- hydroxybenzoate) and we hypothesize that they can also be engineered to work on a broader set of substrates such as benzoate (benzoate TPA). In order to engineer such an enzyme, we developed a TPA biosensor in *Acinetobacter baylyi* ADP1, a versatile soil bacterium for microbial engineering and an industrially relevant strain. Using large libraries of enzyme variants in ADP1 verified in vivo by the TPA biosensor, high throughput screening and selection of carboxylase enzymes capable of performing the desired conversion will be made possible; thus demonstrating the very first example of TPA production from renewable sources.

## **Emmanuel Burns**

Program: UGS/Postbac  
School: Atlanta Metropolitan State College  
Group: B-11  
Mentor: Munehiro Teshima

Category: Biosciences  
Type: Individual  
LA-UR: 19-20742

### **Analysis of rock varnish as a source of biological signatures for Mars extant life.**

Mn is considered a principal biosignature for Mars. The most common terrestrial Mn-rich surface material on Earth is desert varnish, a dark, shiny coating on rocks. Microbes occupy within rock varnish, and it is probable that the concentration of Mn in rock varnishes is mediated by microbial activity. Here we report research aimed at 1) identifying and interpreting the microbial species and processes involved in the habitation and/or formation of rock varnish, and 2) identification of organic biosignatures that, in concert with trace element and mineralogy, can be used to conclusively distinguish the biogenic and abiogenic origins of terrestrial Mn-rich surfaces so that we may then apply the knowledge gained in this work to martian datasets from ChemCam and SuperCam. We seek to identify unique and/or important organic biosignatures present in varnish. To do this, we have begun characterizing the organic materials using LC- QExactive with Nanomate LESA+ to extract and analyze the organic materials on the rock varnish. In addition, we have isolated microorganisms from varnished rocks, grew them on Mn-rich agar plates and analyzed by LESA+LC-MS. Our overall plan includes the parallel analysis of samples to acquire molecular signatures utilizing Raman and Laser-induced breakdown spectroscopy (LIBS). Create an orthologous database of chemical and mineralogy signatures equivalent to that obtained from the Mars rovers (using ChemCam and the upcoming SuperCam), and correlate to our MS results from terrestrial samples. Examples of metabolites linked to biological pathways that were identified on the surface of the rock include: a) glutathione disulfide, a key metabolite for desiccation resistance in fungi and bacteria, b) organic acids, which are key metal chelators and weathering agents produced by microbes, and c) a variety of amino acids. We aim to discover terrestrial biosignatures that could be characterized and associated with signatures detected in Mn-rich rocks on Mars.

## **Elisa Cirigliano**

Program: UGS/Postbac  
School: University of British Columbia  
Group: B-11  
Mentor: Taraka Dale

Category: Biosciences  
Type: Individual  
LA-UR: 19-26383

### **Cryopreservation as a method of long term storage for microalgae**

Cryopreservation is the process of freezing biological materials at extremely low temperatures in order to suspend all biological processes, including those that lead to cell death and DNA deterioration. In theory, cryopreservation would allow cells to remain in a frozen state, unchanged, for decades without any damage. Regular freezing can cause crystals to form in and around the cells that can pierce cell walls and cellular tissues. However, cryopreservation involves adding a solvent that is nontoxic to cells, and permeable to the cell wall, so it has access to all parts of the cell. This increases the total concentration of all solutes in the system, which decreases the amount of crystals formed at any temperature.

Cryopreservation is beneficial for long term storage of microalgae because it ensures that the cells remain the same as they were when initially stored. Currently, algae cultures are stored on agar plates and are continuously growing. The cells could be kept this way for years, but over time the cells may change due environmental fluctuations or bacterial interference. Using cryopreservation techniques to store microalgae would help to ensure that a strain of cells that was stored years ago is the same today.

Benefits of cryopreserving cells include being able to repeat experiments or continue in research directions without concern over changing cultures. While there are previously developed protocols for some algae strains in the research community, we need to evaluate these protocols across the specific microalgae strains in our lab. The goal of this project is to develop a protocol (or protocols) for cryopreservation that minimizes damage to the cells, and maximizes cell viability and ability to grow well in media after being cryopreserved.

## **Rachel Frankle**

Program: UGS/Postbac

School: Royal College of Surgeons in Ireland

Group: B-11

Mentor: Jacob Yoder

Category: Biosciences

Type: Individual

LA-UR: 19-25877

### **Metabolite Analysis of Bacterial Biothreats using NMR Spectroscopy**

As pathogenic bacteria continue to evolve and develop resistance to current antibiotic therapies, health care providers are faced with increasingly deadly and multi-drug resistant bacterial species. Most new antibiotics resemble current ones, both in structure and mechanism of action; hence, bacteria quickly adapt to these new drugs, and resistance often emerges during clinical trials before the drugs become commercially available. Therefore, the need to discover novel antibiotic pathways and targets is paramount to patient treatment and human health. To accomplish this, we examine amino acid and metabolite uptake by pathogenic bacterial species to determine the metabolic needs of the bacteria, in particular the changes in metabolism resulting from applied antibiotic stress. To determine which metabolites are taken up/released by each species and in what concentrations, we employ nuclear magnetic resonance (NMR) spectroscopy. Each amino acid and metabolite has a unique spectral fingerprint that we use for identification, and spectral peak height yields quantitative information. Thus, principle component analysis of the spectra enables us to determine the amount of each metabolite taken up/produced by the bacteria under various environmental conditions. The bacteria are expected to show increased uptake of amino acids and elevated production of certain metabolites when stressed via antibiotics. As the pathogens must alter their metabolism when exposed to antibiotics, the transport proteins for these molecules will serve as novel targets for antibiotics and will direct future drug development. By establishing the metabolites preferentially consumed and produced during antibiotic stress, resistance mechanisms will be better understood and allow novel drugs to be developed without the fear of existing resistance mechanisms.



## **Estrella Gonzalez**

Program: UGS/Postbac

School: University of New Mexico

Group: B-10

Mentor: Armand Dichosa

Category: Biosciences

Type: Individual

LA-UR: 19-26953

### **Linking evolutionary speciation and behavioral traits in *Cyprinodon* spp. fish utilizing next gen sequencing of the gut microbiome**

Despite making up nearly 50% of all vertebrates, very few microbiome related studies have been performed on fish. To our knowledge, no study has attempted to correlate changes in the diversity of the gut microbiome community to the evolutionary lineage of fish speciation. Conceivably, studying the gut microbiome of fish and its relation to a taxonomic clade that exhibits extremely fast diversification rates will provide a greater understanding of how the microbiome may be a function of the evolutionary lineage. Because microbes can influence reproductive patterns, nutrient absorption, development, and overall health of organisms, I have chosen to test my hypothesis on three species of *Cyprinodon*, and further study how these behaviors may contrast between species. As the gut microbiome diversities in these three species of *Cyprinodon* have not yet been determined, my work seeks to identify how variances in the bacterial populations may relate to their evolutionary lineage. The generalist species (*C. variegatus*) has a diet that consists of a detritus, algae, fish eggs, and plant material. *C. variegatus* is the ancestor of two species that have evolved with jaw morphologies and related specialized diets. The scale-eater or piscivore (*C. desquamator*) and the snail-eater or molluscivore (*C. brontotheriodes*) have evolved within the last 6000 years. My goals are to (1) determine the gut microbiome of the three species and (2) identify how deviations in the microbiome diversity may relate to their evolutionary lineage. To address my hypothesis, I have extracted, quantified, and amplified the bacterial 16S rRNA gene from fecal samples of wild-caught fish for next generation sequencing and EDGE Bioinformatics analyses to determine and compare the bacterial diversities. The results of my work will be the first to link diversification of gut microbiomes with evolutionary speciation, and have implications on how such diversity relates to behavior.

## **Summer Hatmaker**

Program: UGS/Postbac

School: Roane State Community College

Group: B-11

Mentor: John Dunbar

Category: Biosciences

Type: Individual

LA-UR: 19-26482

## **Culturing of Microorganisms that Impact Dissolved Organic Carbon Concentrations in Soil**

Microorganisms are the driving cause in leaf litter decomposition. This is important because they have the ability to correlate with the Dissolved Organic Carbon (DOC) in terrestrial ecosystems. Isolating soil microbial communities can give insight on what microbes have a greater impact on DOC, and can provide directions for future ecosystem manipulations. Being able to target the microbial impacts on the carbon cycle can lead the way to better understanding global modeling. This future modeling technique can give insight on large environmental changes such as climate change. Discovering widespread microbial processes that create variation in soil carbon (C) cycling within ecosystems has the potential to both improve soil C modeling and provide direction for future ecosystem manipulations in C sequestration. Toward this end, in a previous experiment we screened 206 soil communities decomposing plant litter in a common garden microcosm environment and examined features linked to divergent patterns of carbon flow. Carbon flow was measured as carbon dioxide (CO<sub>2</sub>) and dissolved organic carbon (DOC) from 44-days of litter decomposition. Two large groups of microbial communities representing “high” and “low” DOC phenotypes from original soil and 44-day microcosm samples were down-selected for microbial profiling. At a broad scale, we found that bacteria were the strongest drivers of DOC outcomes. However, the physiological mechanisms driving variation in C flow remain elusive. Here, the goal is to gain greater insight into the bacteria associated with the two divergent DOC phenotypes. We are using culturing techniques to isolate bacteria from soils associated with the high and the low DOC community phenotypes. This culture collection will be used as a resource in future studies: 1) focused on identifying bacterial features linked to differences in C flow and 2) focused on building microbial consortia with the potential for increased ability to promote C sequestration in soils.

## **Liam Herndon**

Program: UGS/Postbac

School: Massachusetts Institute of Technology

Group: T-6

Mentor: Sandrasegaram Gnanakaran

Category: Biosciences

Type: Individual

LA-UR: 19-26805

### **Machine Learning to Identify Antibiotics**

With the rise of antibiotic resistance, most infections that have historically been treated with antibiotics now have strains that cannot be treated through traditional antibiotics. This development poses a major threat to public health and national security, and antibiotic-resistant infections are expected to be a leading cause of death in the next two decades. To prevent public health catastrophe, it is critical to discover new antibiotics to replace existing ones as they become obsolete. Antibiotic discovery is, however, an incredibly slow process due to its high failure rate. Every year, out of hundreds of molecules tested, only one or two go on to become antibiotics. This low success rate is caused in part by the difficulty of accurately identifying molecules that can permeate cell membranes and avoid efflux pumps in gram-negative bacteria. To overcome this obstacle, we have developed two machine learning algorithms that can respectively predict membrane permeation and efflux avoidance using a logistic regression of physiochemical and molecular dynamics descriptors. We have used agglomerative clustering to identify highly correlated descriptors, and reduced our set of 155 descriptors to a sets of 5-10 uncorrelated descriptors that produce the most accurate predictions. In addition to the expected physiochemical descriptors describing size and polarity, we have identified several MD descriptors describing interactions with efflux pumps and membrane lipids that can be used to predict permeation and efflux avoidance. This discovery provides unprecedented insight into the specific types of interactions involved in membrane permeation and efflux. Additionally, selected features could be used for a more complex machine learning algorithm in the future, allowing accurate identification of likely membrane permeators and efflux avoiders.

## **Makaela Jones**

Program: UGS/Postbac

School: New Mexico State University

Group: B-11

Mentor: Ramesh Jha

Category: Biosciences

Type: Individual

LA-UR: 19-25863

### **High throughput enzyme design and screening of a monooxygenase for “green” chemicals**

Microbial production of chemicals using renewable substrates (plant biomass) has often been referred to as a sustainable and “green” route. However, microbial production of “green” chemicals is very frequently hampered by bottlenecks in the metabolic pathways. Since the efficiency and productivity from a metabolic pathway is just as good as the slowest step (bottleneck), it necessitates expedited engineering of bottleneck enzymes in the laboratory for improved catalytic efficiency. One such enzyme is p-hydroxybenzoate hydroxylase (PobA), which belongs to the family of monooxygenases and catalyzes the integration of an oxygen atom onto the substrate 4-hydroxybenzoate (4HB) that can be derived from renewable substrates (lignin and sugars). We targeted the PobA enzyme from *Pseudomonas putida* for enhancement of catalytic efficiency, such that the renewable substrates can be diverted to “green” chemicals and plastic precursors via the intermediate protocatechuate (PCA), the product of enzyme PobA. In the interest of enhancing the activity of PobA, combinatorial libraries based on computational prediction were created by diversifying multiple sites in the core of the protein that could provide catalytic advantage to the enzyme. Utilizing a previously developed sensor-reporter system for the product PCA, the libraries of diversity  $10^2$ - $10^5$  were constructed and efficiently screened and selected for high activity, with a goal of relieving the bottleneck in the metabolic pathway.

This internship helped me understand basic components of the living system at the molecular level and provided me with an experience to manipulate their function at my will, produce them in the laboratory set up and select for an improved function, recapitulating the “slow” process of evolution in a matter of weeks.

## **Jared Jurss**

Program: UGS/Postbac  
School: Loyola University Chicago  
Group: B-10  
Mentor: Blake Hovde

Category: Biosciences  
Type: Individual  
LA-UR: 19-25584

## **Computationally Locating Off-Target Effects of CRISPR/Cas9 in Human Embryonic Stem Cells**

The CRISPR/Cas9 gene editing system has become a widespread tool for researchers studying a wide range of topics and species and has opened many doors in the field of genetics, genomics, and public health. One of the main challenges of the system has been the detection and prevention of unintended gene edits when using the CRISPR/Cas9 system to edit genomes. This project focused on developing a bioinformatics tool which can computationally detect off-target edits from CRISPR/Cas9 using short read, next generation sequence data.

In order to computationally determine off-target edits using sequence data the development of a k-mer based analysis tool was necessary. This tool directly compares the k-mers of a control cell and the k-mers of an edited cell on a genome-wide scale. These k-mers are generated from quality filtered raw reads and are filtered based on abundance in both genomes. If a certain abundance of a unique k-mer is determined to be present in the Cas9 edited clone when compared to the un-edited cell line, it may represent a mutated region of the genome caused by a Cas9 mediated event. The unique k-mers are assembled and subsequently mapped to the assembly of the control genome. The regions which have possibly been edited are flagged and the exact nature of the edit is determined by a further k-mer analysis of the region. Any which show the signature of the specific CRISPR/Cas9 edit are flagged and returned as regions of possible off-target damage.

This tool allows researchers to directly compare edited clone cells to the control cells they were edited from. This allows researchers to better develop methods for specific use cases of CRISPR/Cas9 and along with off-target prediction software can be a powerful tool to prevent and mitigate the effects of off-target edits from use of the CRISPR/Cas9 system.

## **Beauty Kolade**

Program: UGS/Postbac

School: City University of New York, Lehman College

Group: B-11/CNLS

Mentor: Jacob Miner

Category: Biosciences

Type: Individual

LA-UR: 19-26990

### **Validating experimental results of Digitoxin using molecular dynamics**

Cardiac glycosides are a class of biomolecules used in the treatment of heart failure. Previous studies involving the use of ion-mobility mass spectrometry (IM-MS) and molecular dynamics (MD) have been conducted on many different classes of biomolecules but have not been specifically focused on these particular molecules. IM-MS is an analytical separation tool that provides structural information of a molecule based on its mobility (a function of mass, charge and shape), while MD is a computational modeling technique that refines the three-dimensional configurations of biomolecules, and their interactions with particles in the solution-phase. Experimental results from our group have shown that a cardiac glycoside of particular interest (digitoxin) displays 3 different arrival times (peaks) in its ion-mobility spectrum. This project focuses on validating these experimental results and determining the specific configurations that represent each arrival time peak. We perform MD simulations at different temperatures and different salt (NaCl) concentrations in order to characterize the range of possible configurations of digitoxin, and to describe the equilibrium distributions of monovalent ions around digitoxin. From our results, we find that a few highly-extended conformations are formed, and that sodium ions predominantly accumulate around the oxygen atoms of the lactone ring. With our approach, we aim to create a library of ion-mobility-based data for cardiac glycosides that other scientists can use to carry out toxicological investigations of unknown compounds.

## **Isabelle Lakis**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: B-11

Mentor: Babetta Marrone

Category: Biosciences

Type: Individual

LA-UR: 19-26281

## **Multifactorial Optimization of Cyanobacterial Polymer Production Platforms**

Cyanobacteria are a promising photosynthetic platform for the production of renewable chemicals, including polymers that can be used as alternatives to petroleum commodities. Certain cyanobacteria can produce polyhydroxyalkanoates (PHAs), which can be processed as potential plastic substitutes with better biodegradability and reduced carbon footprint. The diversity in PHA polymer length and side chains can be leveraged to determine the properties of the bioplastic produced, lending it a broader set of physical characteristics. To harness the potential diversity of PHA polymers and their production in a cyanobacterial host, we are developing machine learning (ML) tools that optimize the design of 'cyanobacterial metabolic precursors' that may comprise a PHA chain. We will use ML to compare inherent features of PHA-producing and non-PHA-producing cyanobacteria to discover and predict factors that impact the production of PHA. To that end, we will integrate large data sets consisting of cyanobacterial protein domains (predicted metabolic capacity using Pfam abundance) and high-throughput physiological screening through Biolog phenotypic microarrays (metabolic plasticity via nutrient uptake). We expect that this approach will provide our ML algorithms with sufficient data to allow predictions about the PHA metabolic machinery, nutrient effects on PHA polymer characteristics, and optimized cyanobacterial growth and PHA biosynthesis. ML predictions may be further validated through genetic engineering and adjustment of growth parameters. We will advance the goal of a circular bioeconomy by leveraging the metabolic diversity of cyanobacteria and implementing ML tools to accelerate the production of renewable polymers.

**Riya Mahesh**

Program: UGS/Postbac

School: UT Austin

Group: T-6

Mentor: Nicolas Hengartner

Category: Biosciences

Type: Individual

LA-UR: 19-26950

## **Genomic Analysis of Cancer Cell Lines Through Deep Learning**

Cancer is the second leading cause of death in the US. Since both the incidence and cure of cancer have a genomic component, there is an opportunity to individualize treatment. To learn how treatment and genomics are linked, the National Cancer Institute (NCI) and other organizations have developed immortal cancer cell lines to systematically test drug response, and related the assays to gene expression data. We seek to classify the cancer cell lines by cancer type using dense neural networks in Keras. The patient tumor data from the Cancer Genome Atlas is the training data and the cancer cell lines from the Broad Institute is the testing data. The input gene expression matrix has many features and a L1 penalty will be applied to the neural network to reduce this number. The results from this model will indicate whether the genetic composition of the cancer cell lines is indicative of the patient tumors. Because drug response data is not available for the patient tumors, we can predict the drug response on the patient tumors based on the cell lines. By analyzing the genetic similarity between the cancer cell lines and the patient tumors, hopefully the goal of personalized medicine can be better suited for cancer treatment.



## **Savannah Martinez**

Program: UGS/Postbac  
School: New Mexico State University  
Group: B-10  
Mentor: Armand Dichosa

Category: Biosciences  
Type: Individual  
LA-UR: 19-26927

### **Generating Genetically Characterized Panels of Antibiotic-Resistant Biothreat Agent Surrogates via Experimental Evolution**

Understanding the genomic evolution toward multidrug resistance is crucial to prepare our nation and its warfighters from the potential threat of infections from drug resistant pathogens that have gained resistance through either natural or engineered means. The rising number of bacterial species acquiring drug resistance poses a threat to human health on a global scale, while the engineered acquisition of drug resistance in bacterial species may impact our national security. Furthermore, our arsenal of already depleted antimicrobial drugs is rapidly losing their efficacy against such pathogens. To prepare our nation from the threat of drug resistant pathogens, we need to better understand the mechanisms that lead to development of antibacterial resistance. This will in turn lead to the development of novel treatment regimens for combating the actual drug resistant pathogens. Here, I present a pipeline designed to generate antimicrobial and multidrug resistant (AMR and MDR, respectively) bacterial surrogate isolates of non-pathogenic surrogates of human pathogens, *Bacillus anthracis* (Ba, anthrax), *Yersinia pestis* (Yp, plague), *Francisella tularensis* (Ft, tularemia). These surrogate strains (Ba Sterne, Yp A1122, Yp KIM06, Yp KIM 10, and Ft LVS) were evolved to be resistant to various antibiotics (doxycycline, ciprofloxacin, tetracycline, chloramphenicol, rifampicin) by exposure to, at least, 3X the initial minimum inhibitory concentration (MIC) to the selected antibiotics. To quantify the increased resistance to the antibiotic(s), we utilized the Etest antibiotic strips in parallel with the BioscreenC automated growth curve method developed at USAMRIID. We will be sequencing these strains to understand how antibiotic resistance evolves. My work focused on the design and integration of LANL's and USAMRIID's respective AMR/MDR evolution protocols, which will also be utilized to validate the AMR/MDR isolates that have already been generated. Our isolates will be accessioned at USAMRIID for genomic analyses and tested against candidate antimicrobial drugs.

## **Samuel Merriman**

Program: UGS/Postbac

School: Missouri University of Science and Technology

Group: B-10

Mentor: Antonietta Lillo

Category: Biosciences

Type: Individual

LA-UR: 19-26439

### **Modern Plague Defense Mechanisms**

*Yersinia pestis* is the main pathogenic bacteria of the bubonic, septicemic, and pneumonic plagues. It is a gram negative, rod-shaped bacteria that can be transferred to humans through the bite of an infected animal or through the air. Due to the effective antibiotics becoming increasingly rare the possibility for it to be weaponized in a multi-antibiotic resistant form, new treatments and diagnostic methods must be researched. Fraction 1 (F1) antigen is a protein produced on the surface of *Y. pestis*, and allows for a bacterium to circumvent the immune system and is commonly found on virulent strains. Eight anti-F1 antibodies for *Y. pestis* were previously isolated from phage display, demonstrating optimal expression and retained immunoreactivity, and were subsequently converted into full length Immunoglobulin G antibodies (IgGs). From there, three antibodies exhibited higher affinity to F1 compared to the other five, and were selected to proceed to epitope binning. Two of the selected antibodies were revealed to bind to the same epitope on F1, and the other bound to an adjacent epitope. This study helped to support these findings and also explored the kinetics of affinity matured antibodies versus the antibodies isolated from phage display.

The parent project for these studies involving radioimmunology therapy for bacteria will also include *Pseudomonas aeruginosa*. For preliminary studies, anti-human antibodies needed to be isolated. This study involved the use of a single-chain antibody shown in literature to bind specifically with protein on the surface of *P. aeruginosa*. This was confirmed by ELISA and is to be made into an IgG. Next, new custom anti-*P. aeruginosa* antibodies were discovered using phage display with whole cells, then further isolated and characterized the single chain antibodies using flow cytometry and yeast display.

## **Makenzie Quintana**

Program: UGS/Postbac  
School: New Mexico State University  
Group: EPC-ES  
Mentor: Audrey Sanchez

Category: Biosciences  
Type: Individual  
LA-UR: 19-26454

## **Large Game Distribution Camera Study at Los Alamos National Laboratory**

The unique habitats at the Laboratory support a diverse community of wildlife. The habitat types that include Pinon Juniper, Ponderosa Pine, and Mixed-conifer forests each provide different resources important for a variety of species. Wildlife monitoring for large game animals can be challenging because they avoid interactions with humans, and prefer undeveloped areas. This study was conducted to analyze the distribution of predators and other game animals seasonally across the Laboratory. This research informs decisions regarding wildlife management recommendations for conservation and protection. This study utilized game cameras to remotely monitor wildlife. As camera technology has advanced, game cameras have become adequate for documenting individuals, and are commonly used in wildlife studies on predation, abundance, occupancy, diversity, and endangered species detection. Twenty cameras were placed across the LANL landscape using a modified systematic sampling design. They were deployed in February 2018 and retrieved in January 2019, thus each camera sampled for one full year. All images were reviewed and the species, number, age, and sex of all animals in the photo were recorded. Here we present data for the most abundant species encountered: deer, elk, coyote, bear, bobcat, mountain lion, and fox respectively. The data were summarized by species and season. Future work will include occupancy modeling for each species. This will allow the development of heat maps showing species distributions across the Laboratory.

## **Arasely Rodriguez**

Program: UGS/Postbac  
School: Regis University  
Group: B-10  
Mentor: Jennifer Harris

Category: Biosciences  
Type: Individual  
LA-UR: 19-26050

### **Motor Neuron Differentiation from Human Embryonic Stem Cells**

Amyotrophic lateral sclerosis, poliomyelitis, spinal muscular atrophy and other neurodegenerative diseases affect motor neurons (MNs). MNs are an essential part of the nervous system as they control all muscle movement. To study this class of neurodegenerative diseases, a model of human MNs is essential. However, primary human MN cells cannot be expanded and are often contaminated by other cell types. Human embryonic stem cells (hESCs) can be differentiated into any cell type and expanded unlimitedly with better purity, which makes them a valuable tool to research disease and therapeutics. Small signaling molecules can be used to inhibit or activate specific signaling pathways that follow in vivo development of MNs. Thus, I can use these molecules to push hESCs to become MNs. As hESCs differentiate they express different proteins that can be viewed using immunofluorescent staining. Mature neurons should also be electrically active. By directing differentiation, using immunofluorescence, and measuring electrical activity to verify cell identity, I successfully differentiated and validated mature MNs.

## **Kalifa Stringfield**

Program: GRA/Post Masters  
School: Texas A&M University  
Group: B-11  
Mentor: John Dunbar

Category: Biosciences  
Type: Individual  
LA-UR: 19-26051

### **Comparative Genomics of Sulfur Cycling Pathways in Bacteria and Archaea**

All life depends on microbial cycling of elements like carbon, nitrogen, phosphorous, and sulfur. Identifying the participants (microbes) in a particular cycle and their specific roles improves our ability to manage the health of biological systems (e.g. humans or entire ecosystems). We are mapping the microbes that contribute to sulfur cycling by synthesizing data from DOE's large resource of sequenced microbial genomes. Sulfur is essential to the synthesis of many biological macromolecules and is necessary to sustain ecosystems. While all microbes use sulfur as an essential nutrient, some microbes also use inorganic sulfur for energy production. Specific genes are needed for the enzymatic reduction and oxidation reactions of inorganic forms of sulfur; thus, specific genetic pathways are required to carry out these processes. Using the extensive genomic data in DOE's Integrated Microbial Genomes (IMG) database in tandem with the Kyoto Encyclopedia of Genes and Genomes (KEGG), we are mapping the genetic pathways for sulfur metabolism to individual microbes to improve understanding of the distribution of these metabolic capabilities across the bacterial domain — the most diverse domain of organisms on the planet. Our data synthesis allows exploration of constraints on the evolution of these metabolic capabilities and is useful to guide interpretation of the functional processes in complex natural communities. We expect the data synthesis will also identify microbes where new sulfur metabolism genes may yet be discovered.

**Elizabeth Wait**

Program: GRA/Post Masters  
School: University of Texas at Austin  
Group: T-6  
Mentor: Christopher Neale

Category: Biosciences  
Type: Individual  
LA-UR: 19-26798

**Functional Dynamics in a Cancer Protein**

Uncontrolled cell growth can lead to cancer formation. Mutations in Ras, a protein important in growth regulation, can be found in about 30% of human cancers. However, there are still no treatments that target Ras directly. Ras is GTP-activated, but blocking the GTP-binding site is not feasible because GTP binds very strongly and is present at higher concentrations in the cell than any drug could be. A drug would instead have to act at another site on the protein that communicates with the active site to change activity (i.e., allosteric regulation). Traditional design principles target transient pockets whose stabilities correlate with the active site function. As an alternative approach, we aim to identify correlated protein dynamics as targets for drug design. From 1.5 milliseconds of all-atom simulations, we have quantified dynamic ranges and identified dynamic modes. Knowledge of these dynamic regions and modes will be useful in designing a drug for a previously difficult to target cancer driving protein.

## **Jacquelyn Mettler**

Program: GRA/Post Masters  
School: University of New Mexico  
Group: B-10  
Mentor: Blake Hovde

## **Cassandra Miller**

Program: GRA/Post Masters  
School: University of New Mexico  
Group: B-10  
Mentor: Blake Hovde

Category: Biosciences  
Type: Group  
LA-UR: 19-25791

## **Promoter Library Generation to Improve Genetic Engineering Efforts on an Industrially-Relevant Algae Strain**

In order to achieve target production levels of algal biomass and bioproducts, we need to greatly increase the number of genetically engineered strains being developed. Currently, the algal research community is hindered by the limited number of useful genetic engineering tools, making the development of industrially valuable strains and the bioproducts they would produce difficult. This project aims to improve genetic engineering for algae by developing variable strength, and inducible promoter libraries in a stable Cas9 algal cell line, allowing for more precise and reliable control over gene expression.

Multi-condition (light, nitrogen starvation, temperature) transcriptome analysis of *Nannochloropsis salina* will be utilized to develop a library of variable-strength, constitutive promoters as well as inducible promoters. Screening will be performed via transformation of an expression vector, which contains a candidate promoter preceding the mCherry gene (a red fluorescent protein), into a stable Cas9 *N. salina* cell line. Once promoter expression levels are validated via qPCR and mCherry fluorescence quantification, the rank-ordered promoter library and the inducible promoters will be released to the algal research community through the Greenhouse web portal at [greenhouse.lanl.gov](http://greenhouse.lanl.gov).

# **CHEMISTRY**



## **Phuong Chau**

Program: UGS/Postbac

School: Smith College

Group: T-6

Mentor: Christopher Neale

Category: Chemistry

Type: Individual

LA-UR: 19-26803

### **Machine Learning in Molecular Dynamics Simulation**

Molecular Dynamics (MD) simulation is useful for understanding the molecular structure and dynamics of complex system. However, parameterization for MD is still a burden because it is computationally expensive, not very transferable, and only applicable for non-reactive system.

To overcome these problems with parameterization, we are creating an innovative method that is similarly accurate and much faster than quantum mechanic approaches. Specifically, parameters for point-charge all-atom MD are generated by a machine learning network that is trained on quantum mechanical calculations. We validate the method by comparing the experimental chemical thermodynamic properties to those properties calculated by standard MD and our machine learned parameters.

This research has the potential to revolutionize the field of MD simulation by eliminating computational expense and improving accuracy in parameterization. Our framework for MD parameterization will accelerate the research efficiency in various fields including but not limit to drug design, materials development, and industrial catalysis.

## **Kevin Glennon**

Program: GRA/Post Masters  
School: Texas A&M University  
Group: C-NR  
Mentor: Evelyn Bond

Category: Chemistry  
Type: Individual  
LA-UR: 19-26324

### **A Forensic Investigation of Legacy Separated Pu at Los Alamos National Laboratory**

A legacy sample of separated super-grade Pu has been identified in the Actinide Research Facility at TA-48 in Los Alamos National Laboratory. The identified sample has no labeling or reference to its chemical history or reactor origin. Due to its high grade of Pu (> 99.8%  $^{239}\text{Pu}$ ), the sample is hypothesized to originate from the X-10 reactor in the Clinton Engineer Works at Oak Ridge during the Manhattan Project. This hypothesis will be tested using both traditional and modern techniques in nuclear forensics. Traditional forensic techniques will include chronometry to determine separation history, and Pu vector measurements to discriminate reactor origin. Modern forensic techniques will include trace metal analysis to determine whether the sample was purified using the bismuth phosphate or PUREX process, and trace fission product analysis to perform a more rigorous reactor origin discrimination.

## **Elizabeth Hjelvik**

Program: GRA/Post Masters  
School: University of Colorado Boulder  
Group: MPA-CINT  
Mentor: Millicent Firestone

Category: Chemistry  
Type: Individual  
LA-UR: 19-26888

### **Fabrication of polymeric ionic liquid membranes for ultrafiltration applications**

Nanoporous thin films have recently become a highly explored research thrust due to the range of applications in areas such as filtration technologies. In particular, ultra-filtration membranes have been of interest due to their ability to allow particles (e.g., viruses) smaller than 20 nm to pass through their pores thus leading to the effective purification of products in industrial separation processes. [1] However, current etching processes that are used to control the structure and size of the membrane's pores produce significant amounts of waste, present safety hazards and are high in cost. [2] In prior work, the self-assembly of amphiphilic ionic liquid (IL) monomers in water to form liquid crystal mesophases yielding tunable nanostructured polymer networks featuring 20-30 Å pores was studied. [3] In this work, we are studying the ability to transfer the bulk self-assembly/polymerization of the IL monomers to surface supported films. Specifically, 1-decyl-3-vinylimidazolium bromide monomer is spin coated on solid surfaces (glass or silicon wafers) from dichloromethane solution. The resulting thin films were polymerized via UV irradiation. The self-assembled film is assessed by polarized optical microscopy and grazing incidence small angle X-ray scattering. Profilometry is used to determine film thickness. Molecular information was obtained through the use of infrared spectroscopy. The deposition and self-assembly of IL membranes on solid supports serves as a low cost and low hazard alternative to current membrane production processes.

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## **Bonnie Klamm**

Program: GRA/Post Masters  
School: Florida State University  
Group: C-IIAC  
Mentor: Aaron Tondreau

Category: Chemistry  
Type: Individual  
LA-UR: 19-26717

### **Controlling Lewis Acid Catalysis with Lanthanides to form Bimetallic Complexes**

Lanthanide coordination complexes have been of great interest due to their unique photophysical and magnetic properties. Cryptands and other macrocycle ligands can be designed with variable binding sites and shapes to form lanthanide and actinide coordination complexes with selective properties. The cryptand TPT, synthesized by condensation of 2,6-diformyl-pyridine (dfp) with tris-(2-aminoethyl) amine (tren), and similar derivatives provide a 9-coordinate N-based pocket for binding. Here, a series of multi-dentate, macrocyclic TPT complexes with the lanthanides and actinides have been synthesized and characterized structurally and spectroscopically. Single crystal XRD reveals the ligand to adopt various coordination modes, featuring mono- or bi-metallic complexes across the lanthanide series. Traversing from La - Lu, three different structures are observed, where the larger lanthanides coordinate inside the TPT pocket, and the smaller lanthanides hydrolyze the ligand forming bi-metallic complexes. Americium shows even more diverse behavior, forming a mono-metallic TPT cage complex with an  $\text{Am}(\text{NO}_3)_6$  counter ion.

## **Gabriel Levine**

Program: UGS/Postbac  
School: Trinity University  
Group: C-CDE  
Mentor: Stephen Obrey

Category: Chemistry  
Type: Individual  
LA-UR: 19-26776

### **Modifying Carboxylate-Alumoxane Surfaces with Click Chemistry**

Surface modification is an important area of research in chemistry, as surface modifications can be tuned to improve the solubility and performance of the interior compound across different media. Specifically, it is known that particles of  $\gamma$ -alumina, an aluminum compound with the composition  $\text{AlO}(\text{OH})$ , can be reacted with carboxylic acids to form carboxylate-alumoxanes, wherein the terminal carboxylate oxygens coordinate to aluminum in the  $\gamma$ -alumina. With the carboxylic acid securely attached to the  $\gamma$ -alumina surface, different chemistry can be performed using terminal groups on the other end of the acid. We had the goal of attaching alkyne-containing carboxylic acids to alumina to enable further modifications of the surface via the surface. Click chemistry is known to be a robust class of reactions in chemical synthesis. It typically involves the reaction of an azide with an alkyne in the presence of a catalyst, coupling the two groups via a cycloaddition that yields a triazole, with groups that were attached to the azide and alkyne still present. Click chemistry is advantageous because of its high selectivity and yield. Reported in this poster are our results between the reaction of carboxylic acids with  $\gamma$ -alumina to produce alkyne-containing moieties.

## **Kimberly Lopez**

Program: UGS/Postbac  
School: Northern New Mexico College  
Group: C-IIAC  
Mentor: Andrew Akin

Category: Chemistry  
Type: Individual  
LA-UR: 19-26574

### **Evaluation of Isotope Program Shipping Septa**

The LANL Isotope Program develops new isotopes for medicine, nuclear physics, national security, environmental science and industrial applications. Radioisotopes are shipped in glass vials sealed with a rubber septum and crimp seal. The current septa used to seal shipment vials is a 20mm Polytetrafluoroethylene (PTFE) lined grey butyl rubber septum. Recent LANL lab studies have shown that PTFE exhibits excellent chemical resistance but degradation when exposed to high levels of radiation. In order to study the stability and integrity of septa during radioisotope shipment, literature research and laboratory research were conducted. A decision matrix was created to document various 20mm crimp seal septas. We examined chemical compatibility, resistance to HCl, and resistance to gamma radiation exposure. From this matrix of commercially available materials, butyl rubber septas are the most ideal. Full scale testing was then performed and evaluated using the butyl rubber septum. It was found that the butyl rubber septum was compatible at 5 mL of 0.1M HCl for 40 days and greater than 5kGy of gamma radiation.

## **James Louis Jean**

Program: GRA/Post Masters  
School: University of Nevada Las Vegas  
Group: C-NR  
Mentor: Jeremy Inglis

Category: Chemistry  
Type: Individual  
LA-UR: 18-28967

### **Analysis of Uranium and Samarium Isotopic Ratios by Thermal Ionization Mass Spectrometry (TIMS) for Nuclear Forensic Analysis**

Nuclear forensic relies on the characterization of nuclear and radioactive materials to provide information regarding physical and chemical characteristics of samples of interest. Available analytical techniques used in nuclear forensics are classified as Destructive Assay (DA) and Non-Destructive Assay (NDA). Both DA and NDA are critical in responding to environmental release of radioactive material, age, and origin, material trafficking, verifications, treaties, and violations.

After the discovery of nuclear fission by Otto Hahn in 1937 and immediately after World War II, uranium has been used as nuclear fuel to produce electricity and high explosive in nuclear weapons. The contemporary uses of uranium rely on its nuclear properties as  $^{235}\text{U}$  is the only fissile naturally occurring isotope of uranium. However, these applications require enrichment of the fissile  $^{235}\text{U}$  isotope. Most common nuclear reactors in the United States require the concentration of  $^{235}\text{U}$  between 3.5% and 5% (low enrichment). For nuclear devices, the  $^{235}\text{U}$  concentration is between 95% and higher (weapons grade uranium). During fission, the  $^{235}\text{U}$  atom bombards with neutron, causing its nucleus to split into fragments of smaller mass (fission products), releasing energy and additional neutrons, and producing various rare earth elements (REEs). Among the REEs are Nd, Sm, and Gd which are produced in measurable quantities above non-natural isotopic abundances. Fundamentally, the nuclear properties of several of Sm isotopes make this element unique and remarkably useful for nuclear study and geological processes.

The idea of this project is to (1) synthesize a set of uranium (U) containing compounds that are found throughout the uranium fuel cycle (mining to reprocessing), (2) measure their isotopic ratio using thermal ionization mass spectrometry (TIMS), (3) synthesize  $\text{UF}_4$  using ammonium bifluoride (ABF), (4) study and characterize  $\text{UF}_4$  for potential signatures indicative of chemical process history using DA and NDA, and (5) measure sub-nanogram quantity of Sm (fission product) using TIMS for nuclear forensic analysis.

**Katherine Luebke**

Program: GRA/Post Masters  
School: University of Nevada, Las Vegas  
Group: C-NR  
Mentor: Robert Rundberg

Category: Chemistry  
Type: Individual  
LA-UR: 19-26695

## **Calibration of a HPGe Detector for Use in Gallium Cross Section Measurement**

In order to improve measurement of the  $Ga-69(n,p)Zn-69m$  cross section, a portable HPGe gamma ray spectrometer is necessary. This detector, however, must be calibrated with a standard of known identity and activity before it can be used for gallium measurements. These standards must be the same geometry as the gallium target that will be irradiated and measured. The gallium irradiation will be done with a Cockcroft-Walton accelerator (which has a neutron production chamber) at Sandia National Laboratory. Measurements of the  $Ga-69(n,p)Zn-69m$  cross section have varied by a factor of two. With a calibrated HPGe gamma ray spectrometer, measurement error associated with the neutron dose experienced by the gallium target will be reduced. First, multiple calibration standards will be prepared from cationic and anionic exchange membranes. These membranes (in the form of filter papers, plastic films, and mesh grids) will be cut to precise size and shape to match the gallium targets. Each membrane will then be submersed in a liquid stock solution of known isotopic makeup and activity. The membranes will be dried, and measured on detectors to verify the presence and exact activity of each sample. These will then be used to calibrate the portable HPGe gamma ray spectrometer. It is anticipated that the membranes will function as described, but that the total efficiency of each type of membrane will vary. The types of membranes (cationic exchange vs. anionic exchange, material composition, and brand) will be evaluated based on the overall adsorption of standard from solution as well as quality of final product. The successful membrane samples will be used to calibrate the detector. The HPGe detector will then be available for use during gallium target irradiation.



## **Michael Powell**

Program: GRA/Post Masters

School: Purdue University

Group: M-9

Mentor: Shawn Mcgrane

Category: Chemistry

Type: Individual

LA-UR: 19-25243

## **Ultrafast Shock Induced Mid-Infrared Vibrational Changes in Thin Film Explosives**

There are many chemical reactions and pathways predicted to occur during shock loading of explosive materials. Direct experimental evidence of intermediate formation from shock induced chemistry is very limited. Reactive models can provide insight into the chemistry and physics that occur during shock; however, experiments have typically been on orders of magnitude longer time and length scales resulting in limited direct experimental comparison. This work aims to bridge that gap using ultrafast laser spectroscopies to probe electronic and vibrational functional group changes at comparable time and length scales. Broadband mid- infrared (MIR) and visible (VIS) absorption spectroscopy were performed on shocked thin films of explosives materials. Strong absorbance changes were measured in the MIR with peak disappearance as well as a broad absorptive feature in time. VIS absorbance also showed strong absorbance changes indicating electronic structure changes under shocked loading conditions. These results were compared to reactive molecular dynamics and accelerated chemistry models.

## **Harrison Root**

Program: GRA/Post Masters  
School: University of Texas at Austin  
Group: C-IIAC  
Mentor: Stosh Kozimor

Category: Chemistry  
Type: Individual  
LA-UR: 19-26881

### **Expanded Porphyrins and their f-Element Complexes**

Expanded porphyrins are a privileged scaffold within the fields of biology and inorganic chemistry. Their large internal lacuna has proved to aid in the complexation of large metal cations, which are unable to be coordinated by smaller congeners. As such, these scaffolds have the potential to shed light on the properties of f-block elements. Reported herein is the utilization of Schiff-base expanded porphyrins to coordinate the f-block elements in an attempt to understand their unique reactivity and coordination chemistry.

## **Nicholas Starvaggi**

Program: UGS/Postbac  
School: Mount St. Mary's University  
Group: NEN-3  
Mentor: Amanda Graff

Category: Chemistry  
Type: Individual  
LA-UR: 19-26121

### **Giant Quantum Dots as Scintillating Gamma-Radiation Detectors**

This project analyzes the effects of incorporating LANL-patented giant quantum dots (gQDs) in scintillating gamma-radiation detection applications. A scintillator is any material capable of converting some of the energy of incoming incident particles into low-energy photons in the ultraviolet to visible range. In the field, scintillators are often coupled with additional instrumentation to characterize and quantify radiation intensity. Ideal scintillating materials have a high-Z elemental composition to increase gamma-attenuation and photoelectron production, provide high light yields and short emission decay lifetimes, and are relatively inexpensive to manufacture at the large scale. A number of inorganic metals and organic crystals have illustrated scintillating characteristics, but fail to meet one or more of the necessary criteria. Research has thus shifted towards the possibility of embedding high-Z, nanoengineered semiconductors known as quantum dots in low-cost, polymer matrices like polystyrene (PS) or polyvinyl toluene (PVT). Average quantum dots are limited insofar as they participate in self-attenuation, a phenomenon that contributes to a lower net light yield. However, LANL's gQDs do not illustrate this behavior and are thus a viable alternative. The objective of this study is to develop procedures that allow for high gQD loading into polymers traditionally used in gamma-radiation detection while still maintaining optical clarity. In addition, copolymerization with various acrylate compounds will be explored to improve the durability of the resulting scintillator. All scintillating materials will be characterized via IR spectroscopy, UV-VIS spectrophotometry, and fluorimetry. This research lays the foundation for future work in the additive manufacturing (AM) of gQD pieces for deployment in the field at sites like international border crossings.

## **Selena Staun**

Program: GRA/Post Masters

School: University of California, Santa Barbara

Group: C-IIAC

Mentor: Andrew Gaunt

Category: Chemistry

Type: Individual

LA-UR: 19-26737

### **Assessing Covalency in Transuranic Nitrides**

Nuclear energy is a significant component of electricity production in the United States. Used nuclear fuel, waste from the nuclear fuel reactors, is comprised of uranium, fission products (both stable and highly radioactive), and other actinides (Pu, Np, Am, Cm). Various separation schemes for these different components are being considered as part of possible strategies to process and dispose of this highly radioactive waste. One way to separate lanthanides from actinides (and actinides from each other) is through differences in covalency in the metal-ligand bonding. Experimentally, covalency can be probed by NMR spectroscopy coupled with syntheses and structural characterization of target molecules containing multiple bonds with an inherent degree of covalent character. Synthetic protocols developed for thorium and uranium are being extended to neptunium and plutonium taking advantage of unique radiological facilities at Los Alamos to generate novel examples of rare transuranic molecules containing multiply bonded functionalities, specifically with nitrogen.

## **Skyler Logan Szot**

Program: UGS/Postbac

School: Trinity College

Group: C-AAC

Mentor: Alonso Castro

Category: Chemistry

Type: Individual

LA-UR: 19-25505

## **Actinide Isotopic Analyzer**

The overall goal of this project is to develop a fieldable instrument prototype for the isotopic determination of uranium and plutonium with high sensitivity, resolution, and speed. Our method is based on generating a highly collimated atomic beam by heating the sample up to 2000 °C in a disposable tantalum foil micro-crucible in rough vacuum, and measuring laser absorption through it. A laser beam from a tunable diode laser with a center wavelength selected to match a specific atomic transition is intersected with the collimated atomic beam. By detecting the photon absorption through the atomic beam while rapidly tuning the laser across a series of specific isotopes of a given species, a spectrum showing their relative abundance is obtained. This project investigates the development of an automated data acquisition and instrument control sub-system for the prototype. This sub-system controls the various prototype's components through a LabVIEW-based interface that includes digital I/O and RS-232 lines, and acquisition of high-speed laser spectroscopy data through an analog-to-digital converter. This system is an improvement of the fixed lab-base mass spectrometry because it does not require chemical sample preparation, is much faster, and can be taken to the field. The ultimate goal is to develop a high Technical Readiness Level instrument which can be applied to nuclear forensics and safeguards.

# **COMPUTING**

**Ethan Andersen**

Program: GRA/Post Masters

School: University of Colorado Boulder

Group: T-1

Mentor: Danny Perez

Category: Computing

Type: Individual

LA-UR: 19-25461

## **Extending the timescales of Molecular Dynamics simulations by predicting topological changes**

We speed up long-time molecular dynamics (MD) simulations by computing possible MD state transitions based on topological changes between previously observed transitions. In order to quickly identify topological changes we optimize the VF2 algorithm, a popular graph isomorphism algorithm, to find sub-structure in large MD states. The resulting output will allow us to predict paths to and from unseen states at run-time, which will allow us to optimally allocate resources ahead of time during the simulation. In the future we hope to estimate the probabilities of these transitions in order to further improve speed-up.

## **Robert Chiodi**

Program: GRA/Post Masters

School: Cornell University

Group: CCS-2

Mentor: Peter Brady

Category: Computing

Type: Individual

LA-UR: 19-26229

### **Unsplit Multi-Material Advection for the Truchas Multi-Physics Code**

Casting exotic materials is extremely complicated but is also vital for our national defense. Studying these processes in-situ can be very expensive due to the nature of the materials involved. The Truchas multi-physics code seeks to enable the design of these processes in a more cost-effective manner, while at the same time providing unfettered access to study all areas of the mold as the metal solidifies into its final shape. The simulation of advanced casting processes in complicated mold geometries necessitates the use of unstructured meshes in order to properly resolve the shape of the mold. However, the original phase advection algorithm in Truchas, which is responsible for tracking the flow of the molten metals and other constituent ingredients involved in the casting process, was limited to hexahedron elements. My task this summer has been to alleviate this constraint, allowing Truchas to discretely conserve mass and more accurately transport phase volumes for heterogeneous unstructured meshes. This has been done through the implementation of an unsplit geometric Volume of Fluid method, largely driven by an open-source computational geometry library I have recently developed, the Interface Reconstruction Library (IRL). The new advection algorithm will improve simulation quality through allowing more complex meshes that better conform to the true mold topology. Additionally, the amount of man-hours to produce a computational mesh for these casting simulations should be drastically reduced, with the new access to using tetrahedral, wedge, and pyramidal mesh elements without sacrificing simulation accuracy.



**Mai Dahshan**

Program: GRA/Post Masters

School: Virginia Tech

Group: CCS-7

Mentor: David Rogers, Terece Turton

Category: Computing

Type: Individual

LA-UR: 19-26580

## **Examining the Use of Feature Extraction and Semantic Interaction for uncertainty quantification of Image based Simulation Ensembles**

Scientists run many complex simulations with varying initial conditions, known as 'ensembles', to study and understand the influence and relationships among different models and parameters. Many ensemble visualization and analysis approaches focus on the post-processed simulation ensembles' inputs or / and outputs with little attention to insitu image based (i.e., Cinema) simulations and the effect of human in the analysis loop. Cinema insitu image based approach tries to address the challenges introduced by postprocessing simulation in terms of size, bandwidth, and storage by aligning simulation code with postprocessing tasks. This results in a compressed output that directly stores images from the simulation into an image database. Analyzing and exploring Cinema ensembles is different from traditional ensembles as scientists no longer have full access to their simulation inputs and outputs but to a set of images and / or their corresponding metadata. Our work extends Cinema capabilities by integrating it into GLEE (Graphically Linked Ensemble Explorer), a visualization tool based on semantic interaction, making use of GLEE's capabilities to improve interactive analysis of ensemble data. GLEE is an interactive multiview visualization tool that merges human expertise and intuition with machine learning and statistics allowing scientists to explore, search, filter, and make sense of high dimensional ensembles. The proposed integrated framework will enable scientists to explore, compare, and browse ensemble members, helping them gain deeper insight into where and how interesting patterns/ phenomenon happened, quantify the uncertainty about the ensemble, and accelerate scientific discoveries with minimal data representing the simulation. In this poster, we perform a comparative analysis of various image feature extraction techniques (i.e., visual features and semantic features of global features and local features, and unsupervised deep learning) to investigate the effect of these techniques in enhancing the capabilities of the GLEE's visual analysis process with image-based ensembles.

## Zachary DeStefano

Program: UGS/Postbac  
School: Villanova University  
Group: A  
Mentor: Michael Dixon

Category: Computing  
Type: Individual  
LA-UR: 19-27034

## **NNzkSNARK: An Efficient Implementation Of Secure Neural Network zkSNARKs**

We present an efficient and succinct zero-knowledge proof application using zkSNARKs for the remote verification of the forward-pass execution of a neural network of arbitrary size. This allows for the feed-forward execution of a neural network with hidden inputs and/or model parameters to be remotely verified with a small proof. The prover uses cryptographic primitives to attest to the correctness of the initial input and model parameters and generates a succinct proof that attests to the computation of these primitives and the forward-pass execution of the neural network. The zero-knowledge guarantee allows the prover to hide information about the input and model parameters from the verifier while being able to attest to the correctness of the model's execution. We describe how this approach is useful for various applications such as nuclear treaty verification without the need to disclose sensitive data, security camera auditing without the need to leak footage, and secure patient diagnosis without the need to disclose individually identifiable health information.

We demonstrate an end-to-end implementation of this proof system using these gadgets in libsnark on a neural network for the classification of MNIST handwritten digits. To create this demo, we wrote new gadgets for libsnark that implement fixed point arithmetic, neural network functions, Merkle–Damgård Hash construction, and other cryptographic primitives. We optimized the proof system by implementing the program directly in R1CS which achieves better run-time performance and lower memory usage when compared with existing implementations which compile general programs from C.

## **Callum Farrell**

Program: UGS/Postbac  
School: University of Washington  
Group: XCP-8  
Mentor: Daniel Israel

Category: Computing  
Type: Individual  
LA-UR: 19-26591

### **Verification Methods for Tabular Equations of State in xRAGE**

Hydrocodes (such as xRAGE) rely upon equations of state (EOS) to apply hydrodynamic equations to real-world materials. In many systems of interest, these EOS can be very complex, and their evaluation can result in a significant computational cost. This computational setback can be effectively mitigated by using tabular equations of state (TEOS). These TEOS are constructed by evaluating the EOS for a range of parameters, and storing the results in a table. When a hydrocode is run, instead of evaluating complicated EOS, the results are derived from the table, eliminating computational overhead.

However, these TEOS can have noteworthy drawbacks. In particular, when an EOS is not smooth and continuous – as in regions that include a phase transition – it may not be well represented by a TEOS, as the TEOS may be insufficiently dense as to capture sudden variations. This introduces error into numerical calculations.

This project seeks to quantify and understand how the error introduced by using a TEOS affects the accuracy of xRAGE's outputs. In this project, we compute solutions to simple problems using both an analytic EOS and a TEOS, so that in comparing the results we can isolate the TEOS error. Then by using a variety of methods, the effects of the TEOS are characterized and strategies for mitigation are considered and tested.

**Jamil Gafur**

Program: UGS/Postbac

School: CUNY Lehman College

Group: XCP-8

Mentor: Kyle Hickmann

Category: Computing

Type: Individual

LA-UR: 19-26590

## **Optimizing Beryllium Modeling Parameter using a Gravitational Search Algorithm**

Multi-physics codes for the simulation of flyer plate experiments have many parameters that directly affect a simulation's fit to data. In particular, the Preston Tonks Wallace (PTW) strength model consists of eleven parameters and functions as a strength sub-model in simulations of material impact experiments. Using expert judgment and a Particle Swarm Optimizer (PSO) we traverse the parameter space of the PTW model in order to optimize individual parameters in the model while logging and interpolating the overall parameter space. We developed a Gravitational Search Algorithm that implements Newtonian physics to allow for the minimization of our cost function in the parameter space. In this talk we will discuss the overall implementation, development and results of this project.

## **Michael Gonzales**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: T-5

Mentor: Nathan Lemons

Category: Computing

Type: Individual

LA-UR:

### **Calculating Betweenness Centrality in Real-Time to Understand Possible Paths of an Adversary in a Network**

Analyzing a security threat is becoming a harder problem to solve everyday. With large and continuously changing networks, this problem becomes increasingly difficult to solve. This is a concern with important and secured data. In large networks, tracking the path an adversary would take can be difficult. Understanding where they will go helps to prevent the present threat. Using the method of Kourtellis, Morales, and Bonchi, we can calculate the Betweenness Centrality in real time on an evolving network. This gives us a real time look at what is happening and tells us the important nodes and thus, the most likely nodes the adversary may use to travel in the network. Using this in combination with Jupyter notebooks and NetworkX we can calculate the BC based on shortest paths in the network to predict the most direct path an adversary would take in a network.

**Theodore Gonzales**

Program: UGS/Postbac

School: University of Colorado Boulder

Group: A-4

Mentor: Alia Long

Category: Computing

Type: Individual

LA-UR: 19-27028

## **An Evaluation of Discrete Gaussian Samplers for Lattice-based Cryptography**

Recent advances in quantum computation threaten the security of existing cryptosystems. This threat has led to the need of new quantum-resistant cryptography. A popular and promising candidate for quantum resistance is Learning with Errors based lattice cryptography. The computational hardness of the Learning with Errors problem relies on small noise, often sampled from a discrete Gaussian distribution. Implementing an LWE-based cryptosystem in hardware presents a challenge because, despite typically being able to sample uniform true random numbers, modern hardware, such as FPGAs, CPUs, and ASICs do not have the ability to sample from discrete Gaussian distributions. To address this, we implement two methods of sampling from a discrete Gaussian distribution in Python using a uniform distribution: the Discrete Ziggurat and Knuth-Yao algorithms. We evaluated our implementations by benchmarking memory, speed, and side-channel resistance. We discuss security implications for experimental implementations of LWE-based cryptosystems using these approaches. We also illustrate how these algorithms are vulnerable to timing side-channel attacks. If overlooked, such a vulnerability reveals information regarding the small random noise, which effectively breaks LWE-based encryption schemes.

## **Joseph Gorka**

Program: UGS/Postbac

School: University of Wisconsin-Madison

Group: XCP-8

Mentor: Derek Armstrong

Category: Computing

Type: Individual

LA-UR: 19-26026

### **Deep Neural Networks for the Estimation of HE Fireball Parameters**

Progress has been made on the problem of extracting physical parameters of HE fireballs from FTIR data. Kevin Gross, of AFIT, developed a phenomenological model for HE IR spectra which includes parameters tied to physical characteristics of the explosion. Steven Slagle, choosing not to fit to entire spectra, made use of this model to recover these physical parameters with reasonable accuracy through the intelligent choice and analysis of up to 5 spectral bands. The final part of Slagle's master's thesis concerns the development of an algorithm for the selection of these bands, based only on their ability to produce the correct parameter values rather than any physical rationale. This project seeks to build on the work of both Slagle and Gross, and explore the efficacy of deep neural networks (DNN) for the calculation of 6 physical parameters: temperature, size, soot content, and the concentrations of h<sub>2</sub>o, co<sub>2</sub>, and co gases. This choice of direction is based on the idea that the highly non-linear nature of DNNs are well- suited for the complex relationships between the fireball parameters and the many radiance values along the spectra to which they may be related. Tensorflow is employed for the creation, training and testing of the DNN. The phenomenological model, along with several checks to ensure realism, is used to generate artificial spectra for training and testing purposes. In addition, it is incorporated into the cost function used for the adjustment of network weights. Once trained, the DNN is also tested against real data from Brilliant Flash II.

## **Andrew Hitchcock**

Program: UGS/Postbac  
School: Michigan Technological University  
Group: NIE-CDS  
Mentor: Roy Nielsen

Category: Computing  
Type: Individual  
LA-UR: 19-26702

### **Get Packing!**

Creating virtual machines can be a long and complicated process. When developers need to test something in a specific computer environment, it is almost always tested within a Virtual Machine. Since creating these virtual computers is a complicated and time-consuming process, it can take away from the time allotted for testing and development. This problem increases exponentially when more than one virtual environment is required.

There are several possible solutions to this problem. Currently lab employees and students can request virtual machines using Infrastructure on Demand (IoD), but it can take a day or more to create each machine, and they may not have options to create the operating systems the developer requires. Another solution means having developers manually set up their own virtual machines on local hardware. While faster than ordering a VM from IoD, this still takes valuable time and attention away from development.

This research proposes a much simpler solution. Using software tools like Packer and Vagrant, virtual machine creation can be automated. With these tools virtual machine images can be customized, auto generated, and stored wherever they are needed. Using one of these pre-built virtual machines is as simple as running a single command and watching the process complete by itself in a matter of minutes. When testing is complete, the VM can be completely destroyed with a single command. This process can be repeated as many times as is required with the VM coming up exactly the same each time it is started. Not only is this faster and simpler than any of the options currently available, it is the most consistent testing method for virtual environments to date. Using these tools would allow developers to spend more time actually developing, better contributing to the high standard of scientific excellence here at the laboratory.



## **Haydn Jones**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: A-4

Mentor: Juston Moore

Category: Computing

Type: Individual

LA-UR: 19-26504

### **Robust Detection of Computer Generated Text**

State of the art language models are now capable of generating lengthy, coherent texts after only being fed a short prompt. This could lead to abuses such as automated propaganda/fake-news generation, online impersonation, and more. Techniques are being developed to classify a given text as human or machine written, however, many of these techniques are not robust when it comes to adversarial attacks. This work presents the performance, both in terms of classification accuracy and adversarial robustness, of a sparse-coding based classifier designed to solve this task. It also explores further applications of textual sparse-coding, such as filling in missing words from a document.

## **Anthony Leary**

Program: GRA/Post Masters  
School: University of Central Florida  
Group: XTD-PRI  
Mentor: Eugene Dougherty

Category: Computing  
Type: Individual  
LA-UR: 19-26865

### **CMF Job Control**

The Common Modeling Framework(CMF) acts as an interface to set up, model, and run physics simulations to create visualizations for FLAG and RAGE hydrodynamic code inputs. Modeling authorities included in CMF, such as physvalLAP, and physvalEAP, will use the job control library to write batch scripts using the SLURM Workload Manager (Simple Linux Utility for Resource Management), launch and monitor FLAG jobs, manage restarts, and launch post- processing. The job control library will create a batch script that allocates nodes for a duration of time to perform the job, and manages a queue of pending jobs. Modeling authorities will use the library at their discretion, or a stand-alone run script that will be included. As a demonstration of the capability, we will integrate the job control library with the parameter study capability in CMF that was developed by Kyle Hickmann.

## **Benjamin Mastripolito Wachter**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: NSEC

Mentor: Rao Garimella

Category: Computing

Type: Individual

LA-UR: 19-26745

### **Assessing Data Structures and Loop Ordering on Multi-material Physics Simulations**

We use several performance analysis packages to independently verify the static analysis method of Fogerty et.al. for the assessment of multi-material data structures and computational kernels. Many computational physics problems of interest to LANL have a sparse distribution of several different materials, which leads to considerable challenges in designing efficient data structures. Storing field values for all materials in all cells leads to good scaling but the high memory usage makes them inefficient or even inoperable at high resolutions. To solve this, physics codes use many different compressed data structures that have clear benefits over no memory compression. To compare these data structures effectively, Fogerty et.al. isolated small simple loops and evaluated their efficiency using a static analysis of memory operations in the loops. In this project we use several performance analysis tools to independently verify the analysis done in this paper. Our goal is to determine which of several tools is most fit for assessing the real-world performance of these algorithms, as well as affording an acceptable comparison to the static analysis. The tools work in slightly different ways, and these differences are important in determining their usefulness. For example, two of the tools use CPU hardware counters, which are hardware dependent. Another tool uses semi-static analysis of LLVM intermediate representation to count memory operations. Each tool also has its own unique API and command-line tools. These were all important factors in assessing their effectiveness.

## **Justin Natzic**

Program: UGS/Postbac

School: University of New Mexico

Group: NIE-CDS

Mentor: Margaret Kamphorst

Category: Computing

Type: Individual

LA-UR: 19-26809

### **Model T or Model 3: Visualization of Cybersecurity Vulnerabilities**

One of the many responsibilities of NIE-CDS is to provide metrics pertaining to cybersecurity vulnerabilities. Due to the vast amounts of data NIE-CDS collects, it can be difficult to analyze and visualize the data. Providing the data in a clean and intuitive manner can help LANL IT management make better informed decisions. This is especially useful in recognizing trends and patterns within the data. This research discusses the processes of visually representing LANL cybersecurity vulnerability information and metrics in an aesthetically appealing manner. The implementation of Tableau to better visualize cybersecurity vulnerability data allows IT staff and IT managers to quickly analyze data and make informed risk based decisions.

## **Xiaochen Ni**

Program: UGS/Postbac  
School: University of Chicago  
Group: XTD-PRI  
Mentor: Eugene Dougherty

Category: Computing  
Type: Individual  
LA-UR: 19-26868

### **A ModelViewer for the Common Modelling Framework**

The Common Modelling Framework (CMF) ModelViewer acts as an interface to visualize the modelling parameters for FLAG and RAGE hydrodynamics code inputs. While both FLAG and RAGE are used to solve similar simulations, the physics and infrastructure on which the two codes operate on differ. The CMF project aims to unify the various modelling decisions used in these simulations under different authorities. ModelViewer provides a model and authority agnostic visualization tool for CMF. Using Python, Matplotlib, a Python plotting software, and PyQt4, a graphical user interface (GUI) package, we are able to visualize a 2D model of the materials and their initial conditions and regions. Upon hovering over each region, users can easily see the modelling decisions used for the different materials as well as their initial conditions. ModelViewer works to simplify the user interpretation of input files, which can often be difficult to their order-independent structure. Currently, ModelViewer is implemented for FLAG using a single modelling authority and will be further expanded to include other physics authorities.

**Paula Olaya Garcia**

Program: GRA/Post Masters

School: University of Tennessee, Knoxville

Group: CCS-2

Mentor: Jonas Lippuner

Category: Computing

Type: Individual

LA-UR: 19-27045

## **Benchmarking sparse matrix solvers on CPUs and GPUs for nuclear reaction networks**

Understanding the creation of elements in our solar system requires solving many small sparse linear systems of equations, which can be a key bottleneck for this and many science simulations in other fields, such as astrophysics, neuroscience, graph analysis, machine learning, and quantum chemistry. In this work, we compute the rapid neutron capture process, responsible for the creation of half the elements heavier than iron, using SkyNet, which is a nuclear reaction network that evolves the abundances of elements under the influence of different reactions. The most time consuming stage of the simulation is solving a roughly 8000 x 8000 sparse linear system with only 0.24% non-zero entries. We benchmark both direct and iterative sparse matrix solvers on the CPU and GPU. Specifically, we present time performance comparison between three libraries: MKL, CuSolver and MAGMA. We find that direct solvers are more accurate and robust, but iterative methods are easier to parallelize on modern architectures. Due to the small size of the sparse matrices, the performance is better on the CPU than the GPU for a single system, and hence batching a large number of sparse systems is necessary to obtain good performance on the GPU.

## **Elijah Pelofske**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: CCS-3

Mentor: Hristo Djidjev

Category: Computing

Type: Individual

LA-UR: 19-26705

### **Decomposition Algorithms for Scalable Quantum Annealing**

Commercial adiabatic quantum annealers such as D-Wave 2000Q, which is available at LANL, have the potential to solve important NP-complete optimization problems efficiently. However, one of the primary constraints of such devices is the limited qubit connectivity and the size of the available hardware, which limits the size of the problems solvable on the machine to about 65. This research presents two exact decomposition methods (for the Maximum Clique and the Minimum Vertex Cover problem, two of the most important and well-known NP-hard problems) that allow us to solve problems of arbitrarily large sizes by splitting them up recursively into a series of suitably small subproblems. Those subproblems can then be solved exactly or approximately by a quantum annealer and their solutions can be combined into a solution of the original problem. Previous approaches were based on heuristics and could not guarantee optimality of the solution or estimate the error of approximation. In contrast, our decomposition algorithms have the property that the optimal solution of the input problem can be reconstructed given all generated subproblems are solved optimally as well. We present a study of various heuristic and exact bounds as well as reduction algorithms that help to increase scalability of our decomposition algorithms.

**Joanna Piotrowska**

Program: GRA/Post Masters  
School: University of Cambridge  
Group: T-CNLS  
Mentor: Jonah Miller

Category: Computing  
Type: Individual  
LA-UR: 19-26740

## **Spectral shock detection in dynamically developing discontinuities**

The accurate and efficient solution of partial differential equations is crucial for understanding complex physical problems. Pseudospectral schemes are a class of numerical methods successful at solving smooth problems with high accuracy due to their exponential convergence to the true solution. Unfortunately, when applied to discontinuous problems, such as fluid shocks and material interfaces, pseudospectral solutions lose their superb convergence and suffer from spurious oscillations across the entire computational domain owing to the Gibbs' phenomenon. Luckily, there exist theoretical remedies for these issues which were successfully tested in practice for cases of well defined discontinuities. However, realistic applications require treatment of discontinuities dynamically developing in time, which pose challenges associated with shock detection. More specifically, smoothly steepening gradients in the solution spawn spurious oscillations due to insufficient resolution, causing premature shock identification and information loss. We improve the existing spectral shock detection techniques such that they allow us to automatically detect true discontinuities and identify cases for which post-processing is required to suppress spurious oscillations resulting from the loss of resolution. We then apply these techniques to solve an inviscid Burgers' equation in 1D, demonstrating that our method correctly treats genuine shocks caused by wavebreaking and removes oscillations caused by numerical constraints. This is a promising demonstration of the application of pseudospectral methods to problems involving dynamically developing shocks. Our work thus offers a powerful alternative to commonly applied finite volume schemes in accuracy and computational cost.



## **Brian Romero**

Program: GRA/Post Masters  
School: University of New Mexico  
Group: NSEC  
Mentor: John Reisner

Category: Computing  
Type: Individual  
LA-UR: 19-26882

### **Enabling Performance Portable Exascale Atmospheric Simulations**

The utility of computational simulations for large scale atmospheric and multiphysics problems is ever increasing. A necessity exists to provide accurate and timely predictive capabilities to real time events such as wildfires, hurricanes, atmospheric releases and explosions. Coupled to this problem is the diversity of modern computational hardware and the continued demand to adapt code to new architectures. The challenge is the many evolving architectures such as GPGPUs, MICS and multiprocessors. This work describes the effort to port the Fortran code HiGrad to modern, GPU enabled, exascale systems such as the Summit and Sierra supercomputers, the primary feature of which is the NVIDIA Volta GPU. The goals are to reduce the amount of new code that must be written, while utilizing as much of the performance of the new architecture as possible. In this case, the OpenACC framework is implemented and data management is done explicitly through CUDA Fortran device variables. Multi-GPU support is enabled through MPI. Several OpenACC optimization strategies are used including explicit data management, work scheduling optimization and asynchronous threading. The OpenACC tile clause is evaluated for different tile dimensions, and various tile scheduling strategies are tested. To date, single GPU speed-ups of 35x over the original serial CPU implementation have been achieved. Scaling benchmarks, and several other performance metrics are presented. A performance portability metric comparing the CPU, OpenMP and OpenACC implementations is computed over a variety of architectures.

**Boqian Shen**

Program: GRA/Post Masters

School: Rice University

Group: T-5

Mentor: Chengkun Huang

Category: Computing

Type: Individual

LA-UR: 19-26974

## **Accurate and Efficient Numerical Method for the Computation of Synchrotron Radiation in the Near-Field**

The purpose of this work is to develop an accurate and efficient numerical method for the computation of synchrotron radiation (SR) from relativistic electrons in the near field. The high- brilliance electron beam and coherent short wavelength light source provide a powerful method to understand the microscopic structure and dynamics of materials. Such method supports a wide range of applications including material physics, structural biology and medicine development. To understand the interaction between electron beam and synchrotron radiation an accurate and efficient numerical simulation is needed. We compute the radiation near field directly using the Lienard-Wiechert method. Here we present SR simulation results in two dimensions with a parallelized Lienard-Wiechert computation kernel.

## **Nigel Tan**

Program: GRA/Post Masters  
School: University of Tennessee Knoxville  
Group: T-5  
Mentor: Guangye Chen

Category: Computing  
Type: Individual  
LA-UR: 19-26992

## **Performance Portable Relativistic Plasma Simulations for the Exascale Era**

High Performance Computing faces many challenges as we step into the exascale era. The exascale system requirements for performance and efficiency forced computer hardware to diversify with different compute accelerators from multiple hardware vendors. The variety of accelerators complicates development and optimization immensely, and several projects exist to try and tackle the performance-portability problem. Most notably, the Kokkos project provides abstractions for parallel execution and data management that help build performance portable applications for current and future platforms. In this work we present a portable high-performance version of the Vector Particle-In-Cell (VPIC) project using Kokkos that is ready for future exascale systems. VPIC is a highly optimized Particle-in-Cell code that runs on various CPU's and Intel's Xeon Phi Knight Landing accelerators. The Kokkos port enables VPIC to run on the next generation of supercomputers, regardless of architecture, without spending time rewriting code for new platforms. These changes allow code users and physicist to focus on scientific research, instead of code development. Performance results show similar speeds compared to the original VPIC code on a 24 core Skylake node (without any GPU acceleration), whereas enabling the code to leverage NVIDIA GPU accelerators (Tesla V100) provides significant further performance benefits. The port achieves near ideal weak scaling on the Summit supercomputer with up to 2,000 nodes and 12,000 Tesla V100s. We will use this portable and performant port as a base for future development and architecture specific optimizations as computer architectures continue to advance.

**Elizabeth Carlson**

Program: GRA/Post Masters  
School: University of Nebraska-Lincoln  
Group: CCS-7  
Mentor: Robert Pavel

**Vasu Jaganath**

Program: GRA/Post Masters  
School: University of Wyoming  
Group: CCS-7  
Mentor: Vinay Ramakrishnaiah

**Jennifer Ranta**

Program: GRA/Post Masters  
School: Michigan State University  
Group: CCS-7  
Mentor: Julien Loiseau

**Rathish Ratnasingam**

Program: GRA/Post Masters  
School: Newcastle University  
Group: CCS-7  
Mentor: Wesley Even

**Nicholas Stegmeier**

Program: GRA/Post Masters  
School: University of Illinois Urbana-Champaign  
Group: CCS-7  
Mentor: Irina Sagert

**Suyash Tandon**

Program: GRA/Post Masters  
School: University of Michigan  
Group: CCS-7  
Mentor: Sam Jones

Category: Computing  
Type: Group  
LA-UR: 19-26801

## **Core-collapse Supernovae Simulations with FleCSPH**

Core-collapse supernovae (CCSNe) are integral to the formation and distribution of heavy elements across the universe. To study these cosmic events, we use FleCSPH, a smooth particle hydrodynamics (SPH) code developed within the Flexible Computational Science Infrastructure (FleCSI) framework. Our goal for this project is twofold: astrophysical and computational. Astrophysically, we study the impact of various shock structures on CCSNe nucleosynthetic yields and distribution of those yields. The functionality of FleCSPH was adapted to simulate CCSNe progenitors by implementing tabular equations of state, evolution of particle electron fraction, a modified particle lattice generation scheme, and energy injection models to emulate revived shocks in CCSNe. Computationally, we improve the performance portability of FleCSPH through the implementation of Kokkos framework for multi-architectural backends that support multi-CPU and/or multi-GPU systems. Furthermore, FleCSPH and its dependencies are encapsulated in a container using Charliecloud, which allows lean image creation with rootless access to image modifications. Computationally intensive problems such as CCSNe simulations are enabled by exploiting the latest advances in high performance computing hardware and software, highlighting the need for performance portability.

## **Sofia Helpert**

Program: UGS/Postbac  
School: University of Texas at Austin  
Group: CCS-6  
Mentor: Earl Lawrence

## **Yeawon Yoo**

Program: GRA/Post Masters  
School: Arizona State University  
Group: CCS-6  
Mentor: Earl Lawrence

Category: Computing  
Type: Group  
LA-UR: 19-27096

## **Statistical estimation via Variational Inference using MPI and GPUs**

Large-scale simulations, like those used in climate, produce huge data sets. Since writing these to disk is very slow, our goal is to analyze this data within the simulation. This approach is known as in-situ analysis. Bayesian statistical analysis involves determining probability distributions of the model parameters of interest. Accurate solutions can be found using Markov Chain Monte Carlo, however, this method is too slow to be used in-situ. Instead, variational inference is an optimization technique that finds the best approximation to the actual distribution, and is less computationally expensive than MCMC. In this project, we develop algorithms using MPI and GPUs to perform variational inference for two important statistical models. MPI is used for t regression to handle the case where data is distributed across nodes. Computations on the GPU are used to speed up the bottleneck linear algebra required for Gaussian process regression. These approaches will become important building blocks for in-situ statistical estimation.

## **Qun Liu**

Program: GRA/Post Masters  
School: Louisiana State University  
Group: CCS-7  
Mentor: Ayan Biswas

## **Subhashis Hazarika**

Program: GRA/Post Masters  
School: Ohio State University  
Group: CCS-7  
Mentor: Ayan Biswas

Category: Computing  
Type: Group  
LA-UR: 19-26861

# **Deep Learning-Based Feature-Aware Data Modeling for Multiphase Simulations**

Data modeling and reduction in In-Situ processing is still facing challenges. A hybrid paradigm of data reduction and feature analysis in the era of in-situ has been overlooked. This paper introduced a workflow for In-Situ data processing and analysis and conducted initial efforts on using Autoencoder for learning and compressing data, it further integrated skip connections for performance improvements. Our experiments demonstrated the effectiveness of the proposed framework, and it can compress data into \$758\$ Bytes from \$226\$ MB per timestep 3D volume.

# **EARTH & SPACE SCIENCES**



## **Siddhartha Bishnu**

Program: GRA/Post Masters  
School: Florida State University  
Group: CCS-2  
Mentor: Mark Peterson

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-23342

### **Optimization of Split-Explicit Time-Stepping Algorithm in MPAS-O**

Ocean models permit a wide range of time scales with the speed of surface gravity waves being  $\sim 100$  m/s while that of the surface currents and internal gravity waves being two orders of magnitude less. It is not practical to advance the full 3D momentum equations with the smallest time step corresponding to the fastest waves due to the computational weight of the problem. So, a traditional approach is to split the momentum equations into two parts, a barotropic part for solving the depth independent fast 2D barotropic waves and a baroclinic part for solving the much slower 3D baroclinic waves. My research involves improving this barotropic-baroclinic splitting of the time-stepping algorithm of the Model for Prediction Across Scales - Ocean (MPAS- O) with a view to improving the stability and solution accuracy without compromising the computational time. More specifically, I have been studying (a) different filters for time-averaging the intermediate instantaneous barotropic modes and including the 'mean' solution in the time derivative for the next baroclinic (large) time step, and (b) different time-stepping algorithms for advancing these barotropic modes. I have programmed a one-dimensional shallow water equation solver in object-oriented Python for simulating the propagation of a surface gravity wave, where I have tested some of these filters and time-stepping schemes. In this poster, I will compare the efficiency of these filters and time-stepping algorithms with respect to the solution error norm and choose the optimum ones to be incorporated in the MPAS-O code base.

**Daniel Castano**

Program: UGSs/Postbac

School: Northern Arizona University

Group: EES-16

Mentor: Alexander Josephson

Category: Earth & Space Sciences

Type: Individual

LA-UR: 19-26188

## **Comparing Emission Profiles of Wildfires vs. Controlled fires in the Chaparral and Eglin Landscapes**

Implementing controlled burns in areas with low fuel moisture and high fuel density can be challenging, as it can result in the controlled fire escalating to a dangerous wildfire. The purpose of this project is to compare the emission profiles of prescribed fires and wildfires, through simulation, by analyzing the mass of soot produced, particle size distribution, and lofting potential between the types of fire. The two landscapes being simulated are a chaparral field in California and a semi-tropical conifer forest in Eglin, Florida, where Florida consistently implements prescribed burns and California does not. This study is done by using HPC simulation of FIRETEC.

## **Brandon Crawford**

Program: GRA/Post Masters  
School: Idaho State University  
Group: EES-14  
Mentor: Emily Schultz-Fellenz

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-26777

### **Small scale surface change detection from UAS photogrammetry**

The ability to detect small scale (<3cm) surface topographic changes over broad-scale areas (100s of meters) is important for multiple fields of study. In addition, the ability to detect and locate underground explosions requires the ability to detect small scale changes among a noisy background. Recently, the use of Unmanned Aircraft System (UAS) with attached camera, in conjunction with surface from motion photogrammetry (SFM), has provided an emergent solution to identifying these small scale changes. However, a large portion of the rapidly growing field of SFM photogrammetry surface change research has failed to account for potential errors in data collection, SFM software constraints, and overall accuracy associated with the number and accuracy of ground control point surveying. Our research team recently acquired UAS-based photogrammetry data at the Nevada National Security Site as part of an NNSA project to improve the United States' explosion detection capabilities by observing and quantifying small-scale ground surface changes related to underground conventional explosions. This work used carefully designed flight parameters, extensive ground control point surveying, and accuracy assessments of input field data and model outputs to achieve improved control on the resolution and accuracy of our research. These combined methods allow for increased confidence that our models reflect the true ground surface which, allows for more precise understanding of real small scale change. This work provides a framework for future research requiring a focus on high resolution surface model creation and surface change detection.

**Isaac Foli**

Program: GRA/Post Masters  
School: New Mexico Institute of Mining and Technology  
Group: EES-14  
Mentor: Gilles Bussod

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-25709

## **Subsurface Actinide Transport: Geologic Framework Model Development - Negev Desert, Israel**

The safe storage of nuclear waste is a critical problem for the modern world. Increasing demand for energy and responsible environmental management places strict parameters on suitability for potential nuclear waste disposal and repository design.

As part of a NNSA-IAEC collaborative US-Israeli project, scientists at LANL and Israel are looking into the suitability of the Negev desert subsurface for the containment of radioactive waste. The geographic isolation, arid climatic conditions and deep (~500m) water table of the NE Negev desert point to the viability of a potential natural barrier to radionuclide migration within a large vadose zone. The Yamin Plain unsaturated zone in the Negev consists of a stratigraphic succession of terrestrial alluvial deposits underlain by impermeable and permeable layers of Late Cretaceous shallow marine sediments of bituminous marls, cherts, and phosphorites. Hydrologic and geochemical experiments performed at LANL on these shallow marine rock samples collected from the Negev desert demonstrate that under certain conditions, these rock lithologies have high actinide sorption capacities.

In the context of the tectonic evolution of the northeastern Negev desert over the past 40Ma, and constraints from outcrop exposures, wellbores and geophysical data we are building a conceptual Geologic Framework Model (GFM) of the Negev subsurface to be used as the basis for flow and transport models. Preliminary results inform us that the mineralogy and geologic structure of the NE Negev subsurface is conducive to the formation of a layered natural barrier to radionuclide migration.

Current and future efforts are focused on the creation of a 3-D computational mesh for hydro-geochemical simulations that evaluate the movement of fluid in the subsurface and the retardation of soluble actinide elements during contaminant migration from a potential repository source.

## **Sarah Greer**

Program: GRA/Post Masters  
School: Massachusetts Institute of Technology  
Group: EES-16  
Mentor: Daniel O'Malley

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-2648

### **Solving a hydrologic inverse problem using a quantum annealer**

Quantum computing has advanced enough that solving basic inverse problems in fields of interest may be beneficial to show proof-of-concept results. The problems solved should be simple enough to work with the current early state of quantum computing hardware, which would be comparable to problems solved in the early stages of classical computing. We use LANL's D-Wave 2000Q quantum annealer to solve an indirect hydrologic inverse problem. In this problem, we have a synthetic survey where hydrologic head measurements are taken at regular intervals over an area of interest. We then use these measurements to invert for subsurface permeability over the survey area, where our model is constrained such that each permeability mesh node can take one of two known values. We invert for the model iteratively, where each model update takes the form of a quadratically unconstrained binary optimization problem which can be solved on the quantum annealer. Successfully solving problems of this type may help establish the importance of quantum computing for the future of hydrologic inverse analysis.

## **Rose Harris**

Program: GRA/Post Masters  
School: University of New Mexico  
Group: EES-14  
Mentor: Emily Kluk

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-25825

### **Soil and Groundwater Characterization at Aloha Acres Farm in Ojo Caliente, New Mexico**

Aloha Acres is a small family farm in Ojo Caliente, New Mexico. Farmer Randy Haynes of Aloha Acres reached out to the New Mexico Small Business Assistance (NMSBA) Program at the lab for help figuring out why his pea plants are yellowing, while his other crops (mixed greens, radishes, etc.) are growing. A visit to Aloha Acres revealed that the farm is split into two geologic units, Qayh and Qayl. These units were mapped and named by the United States Geological Survey (USGS). At Aloha Acres, Qayh is a mix of sand, sandy loam, loam, and clay loam. Qayh is where most of the crops are planted, including the pea plants that yellowed and died. Qayh contains visible white crusts, which suggests that the soils are saline. Saline soils have a high salt content which can hinder plant growth. The other geologic unit at Aloha Acres is Qayl. Qayl is at a slightly lower elevation relative to Qayh and is mostly sand with some loam. Qayl does not contain visible white crusts, and pea plants that were planted in Qayl appear to be healthy. Soil and groundwater samples were collected from both geologic units at the farm and are being chemically analyzed. The results of the soil and groundwater analyses will be used to make recommendations to the farmer to increase his crop yield.

## **John Heneghan**

Program: UGS/Postbac  
School: Montana State University  
Group: EES-14  
Mentor: Sanna Sevanto

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-26505

### **Effects of life stage and soil water retention capacity on stomatal closure point in corn (*Zea mays*)**

With increasing global population the demand for secure and stable food sources is rising. Due to climate change driving increasing aridity in the western United States, crops that can tolerate warmer and drier conditions are needed. These conditions mean that plant drought tolerance will be one of its most important traits for its survival. A plant's internal water loss is determined by the transpiration controlled by the opening and closing of the stomata in its leaves. Stomatal closure point, a metric for plant drought tolerance, is the point where water content inside of a plant's xylem (water transport tissue) is too low for the stomata to remain open to intake carbon dioxide (CO<sub>2</sub>), lest the plant lose all its water to the outside environment. We demonstrate through measurements of soil moisture, rates of photosynthesis, and tissue water content, how the stomatal closure point of corn (*Zea mays*) changes both within the same plant during different life stages as well as between individual plants based off of the soil water retention capacity of their respective soils. This research can be combined with an analysis of the root associated microbial community for each individual plant in order to assess microbial influences on stomatal closure point. Successive generations of *Z. mays* can then be inoculated with these identified microbial communities in order to experimentally determine if the stomatal closure point of *Z. mays* can be pushed in the directions of more or less negative hydraulic conductivity via the plant microbe interactions.

**Kristin Hoch**

Program: UGS/Postbac

School: Earth & Space Sciences

Group: CCS-2

Mentor: Michael Peterson

Category: Earth & Space Sciences

Type: Individual

LA-UR: 19-26602

## **Variable Resolution Mesh Characterization for North American Coastal Simulations with MPAS-Ocean**

Climate model components on unstructured meshes enable variable-resolution, regionally enhanced simulations within global domains. Here we investigate the relationship between mesh quality and simulation statistics using the JIGSAW unstructured Voronoi tessellation mesh generator and the Model for Prediction Across Scales-Ocean (MPAS-Ocean). In the reference configuration, the refined region uses 8 km cells that extend 400km from the coast of North America, within a global low-resolution domain of 30 to 60km cells. Three sensitivity tests are conducted: the meshes are intentionally degraded so that horizontal cells are further from regular polygons; the transition region from high to low resolution is steepened; and resolution of the coastal region is varied from 30 km to 8km. Overall the ocean simulations are robust to alterations in the details of the mesh. Regionally-refined simulations produce coastal transports and eddy kinetic energy that are similar to simulations with high resolution throughout the North Atlantic. These results are useful for setting design criteria for variable-resolution climate model domains.



## **Alexandra Iezzi**

Program: GRA/Post Masters  
School: University of Alaska Fairbanks  
Group: EES-17  
Mentor: Philip Blom

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-26089

### **Underground Explosion Source Modelling Using the Rayleigh Integral**

Detecting and characterizing underground nuclear tests requires numerical and physics-based techniques that can be applied to a variety of geologic areas, explosion depth, and yields. The Source Physics Experiment (SPE) aims to achieve these goals through direct study of underground chemical explosions. Phase 1 of SPE consisted of a series of 6 explosions in granite at the Nevada National Security Site that were densely monitored by seismic, acoustic, and other sensor types. The SPE explosions ranged in depth from 31 to 87 meters with yields between 89 and 5,000 kg of equivalent TNT. Accelerometers were placed near ground zero to record the ground motion during each of the detonations and acoustic sensors were placed in 4-element arrays at varying distances from the source (1-5 km). Here, we build upon the methods of Jones et al. (2015) using the Rayleigh integral approximation to relate the surface motion above the explosion source to the generation of an acoustic signal. We compare our model to the accelerometer and acoustic data collected in the field for each of the 6 shots and investigate the dependence of acoustic signatures on source depth and explosive yield. This is a step towards developing an analysis capability to related acoustic signatures to the induced ground motion and from that to the underground explosive source that produced the ground motion.

Jones, K.R., Whitaker, R.W., and Arrowsmith, S.J. (2015), Modelling infrasound signal generation from two underground explosions at the Source Physics Experiment using the Rayleigh integral. *Geophysical Journal International*.

## **Megan Kaye**

Program: UGS/Postbac

School: Harvey Mudd College

Group: ISR-2

Mentor: Nina Lanza

Category: Earth & Space Science

Type: Individual

LA-UR: 19-26312

## **Visualizing ChemCam Spectral Data Trends Using Machine Learning: Discovering Rock Coatings on Mars**

ChemCam is an instrument on the Curiosity Mars rover that uses an ablation spectroscopy technique called laser-induced breakdown spectroscopy (LIBS) to measure rock and soil compositions on the Martian surface. LIBS uses a pulsed laser to generate a plasma that emits photons at characteristic wavelengths depending on the elements present in the target. Each pulse of the laser generates a single spectrum (~6000 channels), and a typical ChemCam analysis obtains 30 pulses (spectra) on a single location and 5-10 locations per target. Multiple pulses on the same spot generate a depth profile of composition, thereby revealing the difference between the surface and the interior of a target. Such trends are expected in natural rocks that have been exposed to weathering, or dust on the surfaces of rocks also creates a trend with depth. As a result, ChemCam LIBS observations are interrelated at a range of scales and thus are not stand-alone data. The relationships between these related spectra are value to geologists (i.e., domain experts). However, with over 600,000 observations (spectra), it is critical to have advanced data analysis techniques to aid in the assessment of the data for trends of interest. Machine-learning algorithms are a useful tool for finding trends and relationships within the data. Previous work has demonstrated that Gaussian graphical models (GGM) can effectively visualize the relationships between shot-to-shot LIBS observations. Here we apply this previously developed model to new ChemCam data to assess whether model results can be directly tied to geological interpretations. We then describe a novel application of this technique to develop hierarchical structures of GGM across different analysis locations on the same sample to determine whether geologically meaningful relationships are readily discernible.

## **Stephen Kuluris**

Program: GRA/Post Masters  
School: Montana State University  
Group: EES-16  
Mentor: Philip Stauffer

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-26290

# **A Field Scale Modeling Approach for Characterizing Subsurface Radionuclide Movement**

Most power production methods generate waste as a byproduct, which should be minimized and properly controlled. The management of nuclear waste generated by nuclear power plants presents a unique challenge due to the distinct adverse effects of radiation and radionuclides. Isolating and storing nuclear waste deep underground is a potential solution to mitigate these effects but requires characterizing potential flow and transport of radionuclides in the subsurface.

The subsurface of the Nagev desert of Israel has been proposed as a potential nuclear repository site due to its geographic isolation, arid climate and deep vadose zone. Additionally, field observations and lab tests have shown the existence of sorbing lithologic layers that can retard radionuclide movement. To confirm the viability of this repository site, a field scale flow and transport computer simulation is to be employed using PFLOTRAN, to understand the potential movement of nuclear waste through the subsurface.

To build the field scale model, a Geological Framework Model (GFM) is built from known borehole data, outcrop samples and geophysical data. This GFM is used to construct a computational mesh which flow and transport simulations can be run on. Additionally, simulations are populated with physical parameters informed by real-world experimental data and observations. Batch experiments were performed on samples from the sorbing layers to obtain sorption parameters necessary for the simulation. To correctly capture the sorbing capabilities in the simulation, the batch experiments were reproduced using PFLOTRAN using both a linear  $K_d$  model and a surface complexation model. Results show good convergence with experimental data.

In addition to building flow and transport simulations with real-life data, there is also inherent uncertainty in the real world measurements and the spatial geological data within the simulation domain. We investigate ways to quantify this uncertainty using polynomial chaos expansions and sparse grid sampling methods.

**Gabrielle Ledesma**

Program: UGS/Postbac

School: Iowa State University

Group: ISR-2

Mentor: Nina Lanza

Category: Earth & Space Sciences

Type: Individual

LA-UR: 19-26769

**Trace metal associations of Mn-oxides in ChemCam LIBS data to constrain formation pathways of manganese enrichments found in Gale crater, Mars**

Gale Crater on Mars, which once contained a redox-stratified lake, is currently being investigated by NASA's Curiosity Rover. The ChemCam instrument on Curiosity found that ~3% of Gale Crater rocks have manganese abundances greater than ~3 times expected for martian basalt values. On Earth, manganese enrichments can form in aquatic settings as manganese (III, IV) oxides, characteristic of well-oxygenated environments, due to Mn's need for high potential oxidants for oxidation (>>500mV) relative to other redox sensitive elements such as iron. Although present-day conditions on Mars may oxidize iron and sulfur, manganese cannot be oxidized under current conditions. We hypothesize that if the observed martian manganese was precipitated as an oxide, it should be accompanied by other trace elements, as Mn-oxides strongly adsorb trace metals. The suite of trace elements enriched with Mn should inform the formation pathway. The ChemCam engineering model at Los Alamos National Laboratory was used to analyze the elemental composition of Earth lake sediment samples with manganese enrichments which were then compared to ChemCam data. Both Mn-oxide and Mn-carbonates were studied. Samples from Lake Wentworth (MN, USA) and Lake Vermillion (NH, USA) both have ferromagnesian crusts composed of Mn (III, IV) oxides. Manganese (II) carbonate samples include Proterozoic iron formations, ferruginous lake sediments (Lake Malawi, Otter Lake, Brownie Lake). These samples have been analyzed by X-ray fluorescent (XRF) and the mineralogy determined by X-ray powdered diffraction (XRD). Cross plots will be used to compare Earth vs. Mars-based geochemistry data.

**Greta Miller**

Program: UGS/Postbac  
School: Princeton University  
Group: EES-16  
Mentor: Katrina Bennett

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-26899

**Climate Impacts on Infiltration in Northern New Mexico**

Future climate shifts are anticipated to have significant impacts on water resources in the southwestern United States. Understanding how the complex interplay of changes in temperature, precipitation, and vegetation affects the water budget is important for managing regional water resources in northern New Mexico. This study focuses on the application of INFIL, an infiltration model, to the Pajarito Plateau to estimate changes in infiltration and runoff in response to historical and future climate scenarios. The INFIL model was developed using geospatial data including topography, vegetation, soil, and geology information. INFIL was validated against streamflow and groundwater observations, and then forced with four general circulation models (GCMs) representing the range of climate responses for 2040-2069. The results show large uncertainties in the future of the water budget on the Pajarito Plateau, with possible increases or decreases in the modeled infiltration and runoff. The trend towards more arid conditions in the future indicates the need for site-specific adaptations on the Pajarito Plateau and in the surrounding area.

## **Matthew Nellessen**

Program: GRA/Post Masters  
School: University of New Mexico  
Group: ISR-2  
Mentor: Patrick Gasda

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-26543

### **Boron Adsorption In Clay Minerals: Implications for Martian Groundwater Chemistry**

Boron has been detected in Ca-sulfate veins in Gale crater using ChemCam, the elemental composition remote-sensing instrument onboard the NASA Curiosity rover. Borate adsorbs to 2:1 phyllosilicates—dependent on pH conditions. Peak adsorption for most terrestrial clays occurs near pH 9. Curiosity mission results indicate that Gale crater hosted a fluvial lacustrine system in its ancient past. While this study aims to understand borate behavior in martian groundwater, boron also may have been vital for prebiotic processes on Earth and possibly on Mars. Boron stabilizes ribose in solution, which might allow the formation of RNA. The discovery of boron on Mars allows the possibility for RNA-based life to have developed independently on Mars.

We have obtained baseline mineralogy and chemistry for a suite of terrestrial clay samples that includes saponite, nontronite, griffithite, montmorillonite, and talc. We determined our samples to be of variable purity using XRD; the griffithite and saponite both contain plagioclase and pyroxene. We performed preliminary sorption tests on the WMB24b montmorillonite sample at pH 9. While we expected ~500 ppm B adsorption to this sample, 3300–5000 ppm B was detected using LIBS and ICP-OES (Inductively Coupled Plasma – Optical Emission Spectroscopy) techniques. The high amount of B found in this sample indicates some trapped borate crystals may be present. These results will help us refine our future sorption experimental technique. This represents the first boron-clay adsorption experiments for Mars- like clays, which will provide insight on borate behavior in Martian groundwater, improve the quantitative calibration of B using ChemCam, and allow us to infer the amount of boron that may be present in Martian bedrock.

## **John Ortiz**

Program: GRA/Post Masters  
School: John Hopkins University  
Group: EES-16  
Mentor: Dylan Harp

Category: Earth & Space Sciences  
Type: Individual  
LA-UR: 19-26294

### **Noble gas diffusion through variably-saturated rock: implications for verification of subsurface nuclear events**

Gas transport through variably-saturated geologic media has important applications for nuclear nonproliferation, as noble gas detection is one of the best candidates for the verification of clandestine underground nuclear events. The transport properties of porous geologic media with respect to such gases are of fundamental importance in developing accurate predictive transport models to determine the origin of detected nuclear signatures. We therefore aim to characterize the diffusion of gaseous krypton, xenon, and sulfur hexafluoride (SF<sub>6</sub>) through intact porous rock with varying degrees of liquid saturation in order to quantify vapor diffusion coefficients and relate them to changes in rock saturation. We conducted a series of diffusion cell experiments using intact tuff cores at varying saturations. We fit the experimental results using Finite Element Heat and Mass (FEHM) numerical model simulations to calculate effective vapor phase diffusion coefficients for each gas and saturation. Results will be used to develop more accurate transport models for subsurface fission product releases, which have implications for treaty verification, repository science, and radioactive contaminant transport.

## **Samantha Peterson**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: EES-14

Mentor: Emily Kluk

Category: Earth & Space Sciences

Type: Individual

LA-UR: 19-25872

### **Cement fracture sealing methods: self-sealing and smart polymer gels**

Of the various greenhouse gas emissions contributing to climate change, the effects seen by the addition of carbon dioxide to the atmosphere are profound. Carbon sequestration is a method of carbon storage that is being considered as a means to mitigate the effects seen by the large scale release of anthropogenic carbon dioxide into the atmosphere. In order for carbon sequestration to be effective, however, the cement encasing the underground wells that store the gas must be able to withstand time and stress, and this necessitates the need for an effective means of sealing defects in the wellbore cement. In this study, two methods of sealing micro- fractures in cement will be investigated; (1) the self-sealing method, and (2) the injection of a smart polymer gel. The first involves injecting CO<sub>2</sub> saturated water into the fracture to initially induce dissolution of the cement, followed by the subsequent precipitation of calcium carbonates to seal the fracture over time. The second involves the use of an injected pH sensitive polymer gel that can expand to seal a fracture when exposed to acidic conditions produced by leaking CO<sub>2</sub>. Each sealing method will be tested using a high pressure microfluidic pump system to introduce fluid across a sealed and channelized cement chip. Pressure change across the chip and changes in channel geometry will be measured to determine if the channels (representing fractures) have been sealed. Several pressure and temperature conditions will be tested to determine the optimal conditions for each method to be used, and to also provide comparative data to conclude which method of sealing is more effective.



# **ENGINEERING**

## **Megan Armstrong**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: PP-DPSP

Mentor: Jacquelyn Lopez-Barlow

Category: Engineering

Type: Individual

LA-UR: 19-26503

### **Fuel Inventory Model and Fuel Clad Impact Testing**

In order for National Aeronautics and Space Administration (NASA) to complete long duration missions into space, they need a reliable energy source. The Multi-Mission Radioisotope Thermoelectric Generator (MMRTG) is a common energy source for NASA missions. In order for these nuclear batteries to be assembled, Fueled Clads (FC) need to be fabricated at Los Alamos National Laboratory (LANL) for a heat source. For mission planning purposes, it is necessary to ensure that the correct amount of FCs will be manufactured in time to meet the deadline without depleting the inventory of enriched plutonium-238. To aid the success of the FC fabrication campaigns, a fuel inventory model has been developed. This model will help evaluate the amount of plutonium-238 that will be consumed for mission production and safety testing fabrication. The model will be a tool used for planning purposes and will generate an annual report of the inventory for DOE and NASA.

Before sending the MMRTGs into space, the risk of the FC materials failing during possible Earth impact accidents needs to be assessed. Since the 1980s, many different impact tests have been performed to determine the risk of failure given different scenarios. In order to efficiently design future tests, the data from previous tests was collected and analyzed to determine which tests need to be done. This work has been done to help ensure the efficiency, reliability, and the safety of Fueled Clads in MMRTGs for NASA missions.

**Manish Bhattarai**

Program: GRA/Post Masters  
School: University of New Mexico  
Group: CCS-3  
Mentor: Diane Oyen

Category: Engineering  
Type: Individual  
LA-UR: 19-26652

## **Diagram Image Retrieval Using Sketch-Based Deep Learning and Transfer Learning**

Diagrams convey important scientific and technological information, especially in patents. Our goal is to track the spread of technical information by finding copies and modified copies of technical diagrams in patent databases. Standard retrieval methods for diagram images use binary features such as lines, edges, contour, and minor textures for finding similarity but they are not effective in identifying reasonable image matches. Deep learning has proven to be highly successful for natural imagery, but its application to binary imagery has yet to be explored. Diagram images carry little per-pixel information compared to natural images. Image retrieval for scientific drawings and diagrams are difficult to identify using convolutional neural networks (CNNs) due to the simplicity and lack of texture in the image.

We present a deep learning approach that takes advantage of existing large natural image repositories for image search and sketch-based methods applied to binary patent imagery. Current sketch-based methods query similar natural images corresponding to human sketches and drawings. We use deep learning to generate sketches from natural images for image retrieval and then train the retrieval model on the sketches. We then use our small set of manually labeled patent diagram images via transfer learning to adapt the image search from sketches of natural images to diagrams. This framework can work from single shot to zero shot setting meaning queried imagery may have minimal to zero overlap in the training dataset. We can show this holds because of the domain generalization on pretraining the framework from a large sketch set. Our results show the effectiveness of applying machine learning and deep learning techniques for detecting plagiarism in patent images and querying similar images based on the context information.

## **John Daly**

Program: UGS/Postbac  
School: Arizona State University  
Group: NEN-1  
Mentor: Alessandro Catteneo

Category: Engineering  
Type: Individual  
LA-UR: 19-26592

### **CFD Simulations and Validation for Uncertainty Modeling in Ultrasound-based Measurements**

Ultrasonic measurements are commonly used to non-invasively determine the properties of a fluid within a container or a duct. Applications range from taking measurements of specific areas of the cardiovascular system to measuring the temperature of a gas to determining various properties of fluid flowing within a pipe. The speed of sound in a fluid varies with the temperature of the fluid, therefore in order to conduct ultrasonic measurements with minimal uncertainty, the temperature gradient in the fluid along the path of the ultrasonic beam must be known. The goal of this work is to facilitate the development of a non-invasive measurement technique that depends on the speed of sound in a fluid. To this purpose, ANSYS Fluent simulations have been conducted on a geometry representing a cylindrical cavity containing water with natural convection induced by external boundary temperature differences. The results of the simulations were analyzed to determine the temperature gradients present in the fluid, and how those gradients changed with time due to the unsteady flow in the barrel. The results were then used for the purpose of determining the uncertainty present in acoustic measurements of the fluid which were being used to derive additional fluid properties. The model incorporated a transient solver and a density function  $\rho=f(T)$  to accurately simulate the natural convection occurring within the cavity. Time averaged temperature gradients were determined from the unsteady solution and used to determine how the speed of sound would radially vary within the barrel. Accounting for these variations enabled reduction of the uncertainty in the speed of sound measurements, resulting in more accurate estimations of derived properties. Progress has been made to validate the numerical model against experimental temperature measurements.

## **Peter Fickenwirth**

Program: UGS/Postbac  
School: University of Massachusetts Lowell  
Group: NSEC  
Mentor: Adam Wachtor

Category: Engineering  
Type: Individual  
LA-UR: 19-25874

## **In-Situ Ultrasonic Quality Inspection for Metallic Additive Manufacturing**

The recent growth in the metal additive manufacturing (AM) industry and transition of AM parts from prototypes to deployment in service environments has increased the necessity for quality inspection methods of AM parts. Acoustic wavenumber spectroscopy (AWS), a non-destructive evaluation (NDE) technique, was integrated into an EOS M290 powder-bed fusion (PBF) AM machine for performing in-situ quality inspections. AWS utilizes a scanning laser Doppler vibrometer (LDV) to measure the ultrasonic vibration response of the AM parts after each layer is built. The integration allowed the development of 3D NDE volumes and used basic analyses to detect defects. This work details improvements to the integration of the AWS system into the PBF machine from its initial prototype, which enables higher quality data collection and consistent and successful data collection between build layers. Using the higher quality data, more advanced analyses, based on phase and wavenumber, are developed for the data collected from this novel measurement technique. These analyses are then used to identify common defects like delamination, cracking, geometrical defects, and porosity.

## **Kayla Gill**

Program: UGS/Postbac

School: South Dakota School of Mines

Group: AMPP-2

Mentor: Cresta Bateman

Category: Engineering

Type: Individual

LA-UR: 19-26898

### **Recirculating Water System for Metallography**

The current metallography process used to process metals from  $^{238}\text{Pu}$  power sources is an operation with the opportunity for improvement. Water is a vital component to the metallographic grinding process, clearing potentially harmful debris and acting as a lubricant and coolant. The current process requires collection and containerization of water, which is then shipped off as waste. In the presented work, a water recycling system is designed which improves on the old process by recirculating water. This design provides sufficient amounts of water to the grinder without increasing water waste. It includes a pump, filters, and a reservoir. A filter, chosen by micron size exclusion and ease of maintenance, is incorporated to filter out metal particles and grinding media. The filtration process runs on a simple pumping system. The system is also designed to control for cavitation and metal accumulation.

## **Caleb Hatler**

Program: UGS/Postbac  
School: LeTourneau University  
Group: PT-3  
Mentor: Brian O'Neil

Category: Engineering  
Type: Individual  
LA-UR: 19-26685

### **Continuous Robotic Detection of Alpha Radiation Using Four-Bar Linkage Suspension**

Within PF-4, the Los Alamos National Laboratory's plutonium facility, there is a need for faster and more efficient contamination detection. Contamination puts workers at risk and stems from a potential material release within the special gloveboxes. In order to detect contamination faster, the concept for a robotic system that continuously monitors PF-4 was developed. Specifically, this robot would autonomously guide itself through rooms and detect for radiation levels as low as 100 disintegrations per minute (dpm).

The goal of this project is to create a mechanical sweeping system to detect alpha contamination wherever radiological work is done. This system must detect alpha-emitting contamination levels as low as 100 dpm while minimizing the possible spread of alpha-emitting particles. The main design challenge of the system is to keep the footprint of the mobile robot as small as possible while maximizing the robot's speed of detection. The system will additionally need to be serviceable in case of contamination, portable and able to traverse different floor materials, and energy efficient to conserve battery on the mobile robot platform. The system will accomplish this by sweeping the floor with a cloth and measuring the alpha-particles emitted from the cloth. By measuring radiation from the cloth, the robot navigates the building at a reasonable speed while still detecting low levels of alpha-radiation.

## **Sincheng Huang**

Program: IGS/Postbac

School: University of California, San Diego

Group: MPA-11

Mentor: Cristian Pantea

Category: Engineering

Type: Individual

LA-UR: 19-26788

### **Broadband Operation of Acoustic Collimated Beam Source**

MPA-11's Acoustics and Sensor's Team recently developed an Acoustic Collimated Beam (ACCObeam) using the radial modes of a piezoelectric transducer to emit a Bessel beam. By clamping the piezoelectric disk, an extremely powerful low-frequency sound beam can be produced while minimizing unwanted side lobes, thereby producing an acoustic beam that primarily propagates along one direction. Previously, ACCObeam has been explored and characterized for operation at the radial resonances; however, many high-resolution ultrasound imaging applications require broadband signals. Thus, the objective of this research is to explore the broadband characteristics of the ACCObeam. Furthermore, because existing frequency characterization techniques analyze the ultrasound properties one frequency at a time, long measurement times are incurred. In contrast, we investigate multiple frequencies simultaneously by exciting the ACCObeam with a broadband waveform such as a linear chirp or a Gaussian pulse. Subsequent post-processing can extract the beam profile for any specific frequency. We present ACCObeam broadband measurements and compare them to numerical simulation. Additionally, we also discuss the advantages and disadvantages of the broadband waveform data collection technique.



**Laura Inkret**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: Q-17

Mentor: Michael Steinzig

Category: Engineering

Type: Individual

LA-UR: 19-26704

## **Traction-Separation Relationship Between Sylgard-184 and Aluminum Using Double Cantilever Beam Analysis**

The objective of this project is to measure the adhesive strength of Dow Corning's Sylgard- 184 potting material (silicone elastomere) using double cantilever beam (DCB) adhesive testing and digital image correlation (DIC) to measure the small-scale deformations of the potting material. The goal is to validate a traction-separation model to further understand the energy- release rate of Sylgard from an aluminum substrate. Investigators also want to determine if the traction-separation model is dependent upon loading rate and angle of pull.

Investigators are conducting adhesive testing using potting material, Sylgard-184 95:5 and 90:10, and Aluminum cantilever beams measuring 5 in x 0.75 in x 0.25 in. A bond line between two beams is set using 0.020 in thick shims, then Sylgard is injected into the bond line and left to cure for approximately 12 hours. After curing, the shims are removed, a DIC speckling pattern is applied to the DCB specimen, and the specimen is placed in a fixture that is used with a load frame to secure the beams and adjust the angle of pull on the beams. Specimens are pulled apart at two different loading rates (0.03 mm/min, 0.003 mm/min) and three different pull modes (Mode I, Mode II, and Mixed-Mode). Opening displacements of the DCB specimens are measured with DIC cameras, and the results are used to develop a traction-separation model and further understand the debonding properties of Sylgard.

**Melissa Jacquez**

Program: GRA/Post Masters  
School: University of California, Berkeley  
Group: ES-UI  
Mentor: Genna Waldvogel

Category: Engineering  
Type: Individual  
LA-UR: 19-26642

**Permeable Pavement Feasibility and Cost-Benefit Analysis at Los Alamos National Laboratory for Parking Lots and Side Walks**

At Los Alamos National Laboratory (LANL), there are various stormwater management challenges due to the increase of impervious surfaces caused by the creation of parking lots and infrastructure. One of the storm water management techniques to combat these challenges, is to install permeable pavement that reduces overall surface runoff. There is limited stormwater treatment currently at the lab and flooding occurring at building entrances. Both of these concerns can be addressed with permeable pavements. In addition, permeable concrete can reduce the need for other runoff infrastructural projects and it has been proven that permeable pavements speed snow melt while reducing the need of deicing salt. Overall, permeable pavements may be a sustainable solution to LANL's stormwater obstacles.

Although permeable pavements have been successfully in northeastern United States, a feasibility and cost benefit analysis was needed to examine if permeable pavement could be applied at LANL specifically. The study evaluates the feasibility of parking lot and sidewalk alternatives for permeable asphalt in parking lots, pervious concrete, brick pavers, concrete grid pavers, permeable interlocking concrete pavement, and plastic porous grass/aggregate reinforcement. The installation and long term costs are compared to the current construction of storm water designs. The best solutions LANL are detailed in the recommendations.

## **Bailey Kuehl**

Program: UGS/Postbac

School: University of Wisconsin-Madison

Group: MST-8

Mentor: Saryu Fensin

Category: Engineering

Type: Individual

LA-UR: 19-27065

### **Shock Re-compaction of Spall-Damaged Copper**

Dynamic loading of a material often results in spall fracture. When a material undergoes shock compression and is allowed to release, rarefaction waves propagate through the material. If two of these rarefactions intersect, they can create a region of damage through void nucleation and growth called spall. Because of the close relationship between dynamic shock loading and the aerospace and defense industries, the response of a damaged material to a second dynamic loading event is an important concept to understand. Here, we examine the effect of a second shock applied to pre-damaged copper. Spall damage is initially generated through flyer-plate impact experiments, and the resulting materials are then thoroughly characterized. These samples are then subjected to a second flyer-plate impact to examine how the shock interacts with the generated spall region. The double-shocked samples are sectioned to reveal that at relatively modest shock stresses of 2GPa, the pre-existing spall damage is completely re-compacted. Electron microscopy shows that the voids are compacted with enough energy to drive localized recrystallization, effectively welding the material back together to a fully dense state.

## **Andrew Larsen**

Program: UGS/Postbac  
School: Brigham Young University  
Group: NEN-5  
Mentor: Seung Jun Kim

Category: Engineering  
Type: Individual  
LA-UR: 19-26313

## **The Impact of Conjugate Heat Transfer on the VTR Lead Cartridge CFD Model**

The Versatile Test Reactor (VTR) project was launched by the United States Department of Energy in 2017 with the goal of irradiation of materials testing with a fast neutron spectrum for Generation IV reactor applications. The VTR will be a sodium-cooled fast reactor filled with a variety of test cartridges containing non-water coolants such as sodium, lead, molten salt, and gas. The design of each test cartridge requires accurate thermal hydraulic modeling of the internal test coolant; in this case, the test coolant of interest is liquid lead. The cartridge consists of eight material layers which are as follows (from outside moving inward): Stainless Steel 316 (SS316) cartridge wall, liquid sodium coolant, SS316 wall, argon gas insulation, Oxide Dispersion- Strengthen Steel (ODSS) wall, liquid lead down comer channel, ODSS wall, and liquid lead riser channel.

The focus of this poster is to describe the impact of the conjugate heat transfer (CHT) through the insulating layers (the outside SS316, argon, and ODSS layers respectively) on the lead temperature profile in the down comer and riser channels. The modeling software used was Siemens STAR-CCM+ version 2019-R1. The original model did not account for CHT in the outer layers, ignoring thermal interaction between the riser channel and the down comer channel. This fluid-only model results in an underestimation of the thermal profile in the lead loop design. When both solid and fluid were appropriately modeled in the CHT analysis, a temperature discrepancy of 150 °C (compared to non-CHT analysis case) was discovered. As the operating temperature of the proposed Lead-cooled reactor differs from the normal VTR operating condition, and as an accurate thermal profile prediction of the lead loop is one of the key calculations for design optimization, this study will provide methodology development of CHT analysis for high fidelity thermal profile calculations.

**Jerry Li**

Program: UGS/Postbac

School: University of California, Los Angeles

Group: NEN-1

Mentor: Matthew Newell

Category: Engineering

Type: Individual

LA-UR: 19-27043

## **Current to Pulse Converter For Ion Chamber Gross Gamma Measurements**

The Current to Pulse Converter (CPC) is an ideal solution for ion chamber measurement needs when implemented with neutron detector systems. The CPC detects input currents in the range 0.2nA to 2000nA and produces TTL pulses at a rate proportional to the input current, approximately 500cps/nA. Resulting pulses can be counted with any of the existing neutron analysis instruments, e.g. JSR-15. A flickering LED increases intensity with increased input current. The CPC not only simplifies instrumentation needs but also, by using a single counter for both neutron and gamma measurements, time correlates gamma measurement results with the neutron data. The CPC is a simple converter, inexpensive to manufacturer and designed for reliability.

This is an update to an existing design of the CPC. We replaced a voltage to frequency converter with an Field Programmable Gate Array (FPGA) to modernize the circuit and increase the base range of the CPC. Current feeds a transimpedance amplifier which converts the current into a voltage. The voltage is then translated into a digital number using a 12 bit Analog to Digital Converter (ADC). The Xilinx Spartan 7 FPGA reads the digital number and processes it to output a frequency.

**Evan Lucero**

Program: UGS/Postbac  
School: University of New Mexico  
Group: Q-15  
Mentor: Arthur Nobile Jr.

Category: Engineering  
Type: Individual  
LA-UR: 19-26838

**Stress Cushion Material Evaluation**

As part of the B61 LEP, it is important to understand component-, subsystem-, and system-level responses to an in as-assembled state and to define the requirements for Pantex assembly pauses. The stress cushion material evaluation will help to define the amount of time at Pantex an assembly can be left partially assembled without risking next level assembly rejection.

**Sheera Lum**

Program: UGS/Postbac  
School: Mississippi State University  
Group: E-13  
Mentor: Nathan Miller

Category: Engineering  
Type: Individual  
LA-UR: 19-26885

**Characterizing PBX 9502 Ratchet Growth Due to Thermal Effects**

Gaining a better understanding of the ratchet growth of PBX 9502 due to thermal effects is of significant interest to Los Alamos National Laboratory (LANL) analysts. The composite explosive is composed primarily of TATB (1,3,5-triamino-2,4,6-trinitrobenzene), an insensitive high explosive that is known to have highly anisotropic ratchet growth when exposed to extreme thermal environments for prolonged periods. Although extensive ratchet growth testing and analysis has been done for TATB, differing texture and the presence of a polymeric binder in PBX 9502 prevent direct comparison between raw TATB and PBX 9502. Recent test data examining the ratchet growth of PBX 9502 has provided a means for evaluating the ratchet growth model proposed by the Advanced Engineering Analysis Group at LANL. Project tasks for this research have included examining the test data, developing a potential Abaqus model to fit the test data, and performing an uncertainty analysis of the proposed ratchet growth model.

## **Tom Maggiore**

Program: UGS/Postbac  
School: Montana State University  
Group: W-11  
Mentor: Denver Smith

Category: Engineering  
Type: Individual  
LA-UR: 19-26571

### **Transport Container: Phase II**

This spring semester at Montana State University, a group of engineering students were given a capstone project by the W-11 group. This project consisted of designing and creating a transport container for an object that was used at Los Alamos National Lab. The various requirements included maximum dimensions, drop resistibility and weight limitations. While the students did a great job, the container was relatively bulky, and not easy to carry. Phase II of the Transport container consists of a new design with different requirements. One of these new requirements is to utilize the various additive manufacturing processes here at LANL, allowing for a quick turnaround in the creation of prototype parts. Every component of the container, excluding the hardware, will be printed here at Los Alamos National Lab utilizing W-11's print shop. Many different processes employed during Phase II are being used for the first time, so Phase II is not just about a new container iteration, but streamlining and improving multiple processes within the W-11 group.



## **Joseph Mayer**

Program: UGS/Postbac

School: University of Illinois at Urbana-Champaign

Group: P-23

Mentor: John Charonko

Category: Engineering

Type: Individual

LA-UR: 19-25963

### **Molecular Tagging Velocimetry for Shocked Particle Studies**

Knowledge of the unsteady particle kinematics behind a shock wave is important for understanding many flows in extreme environments, such as supernovae and the distribution of blast debris in explosions. However, recent measurements of shock-accelerated particles indicate that drag coefficients are an order of magnitude larger than existing models would predict. This discrepancy cannot be explained by current theory, and simulations in such regimes are extremely challenging. This leaves a need for experimental measurements of the flow around accelerating particles to explain the unknown unsteady effects. Techniques like particle image velocimetry (PIV) are limited by the response time of the tracer particles, so this makes probing the background gas flow around a shock-accelerated particle with PIV impractical. This problem can be overcome using a technique called molecular tagging velocimetry (MTV). In MTV, the flow contains lag-free molecular tracers that are excited by a laser and will continue to emit photons after excitation via phosphorescence. Molecules that exhibit phosphorescence such as acetone and diacetyl are commonly used to seed a gas due to their high vapor pressures and relatively low toxicity. We have chosen to use acetone-based MTV simultaneously with PIV to measure the flow field behind a shock, targeting simultaneous measurement of the particles' motion and the carrier phase gas velocity. The velocity is obtained by calculating the displacement of excited regions of the flow which usually begin as a planar grid of laser lines. To process the gridded images, we have adopted a technique known as the Windowed Fourier Transform (WFT). In this technique, the light intensity of the grid lines is expressed as a periodic signal. Therefore, a slight displacement in the grid can be interpreted as a change in the signal's phase. Implementing MTV for shocked particle experiments is currently underway at LANL's Horizontal Shock Tube facility.

## **Vedant Mehta**

Program: GRA/Post Masters  
School: Georgia Institute of Technology  
Group: NEN-5  
Mentor: Patrick McClure

Category: Engineering  
Type: Individual  
LA-UR: 19-27037

### **Powering the Red Planet in Pursuit of Becoming Interplanetary Species**

Microreactors are state-of-the-art reactor concept with power level rated in-between 1 kWe to 10 MWe. Yttrium-Hydride is being considered as primary moderator for microreactor due to its superior hydrogen containment capability compared to other hydrides. However, as all hydrides, yttrium hydride experiences hydrogen dissociation (and thus losses) at elevated temperatures. This loss affects the neutronics of the system due to the availability of less hydrogen, and hence less moderation. Several material property data is missing for yttrium hydride. In the first part of the study, we investigate material data generation from the first principle quantum mechanical simulations. These properties include thermal scattering laws, diffusion coefficients, heat capacities etc. In parallel, advanced multiphysics simulation techniques are developed to further understand the dependence of neutronics and thermomechanics on hydrogen dissociation. The newly created data from quantum mechanics is then implemented in the advanced multiphysics toolset to properly understand how the microreactor evolves over time. Finally, system optimization is applied to generate the ideal reactor candidate for space applications including nuclear electric propulsion and surface power production. This presentation covers material data generation, benchmark, multiphysics toolset creation, and system optimization.

**Ilyes Mezghani**

Program: GRA/Post Masters

School: UC Louvain

Group: GRA/Post Masters

Mentor: Deepjyoti Deka

Category: Engineering

Type: Individual

LA-UR: 19-26975

## **Robust AC Optimal Power Flow: a Data-Driven Approach**

The optimal power flow (OPF) is a network optimization problem that is routinely solved in power systems operation and planning for determining economic generation dispatch and respecting system constraints. With increasing penetration of renewables and load flexibility, optimal power flow solutions need to be robust to uncertainties in the input conditions.

Robust OPF finds optimal solutions to the OPF problem that are robust against uncertainties in system conditions, in particular in changes in renewable generation and load. Computationally, robust OPF, even in the DC case (which is linear), is hard due to the expansion in number of constraints due to feasibility for all uncertainties within the considered set. This paper presents a data-driven approach to the nonlinear and nonconvex problem of robust AC OPF that optimally uses knowledge of historical data.

In recent work, machine learning methods have been demonstrated to learn the mapping from uncertainty realizations to the optimal solution of the DC OPF. The novelty of the approach is that instead of learning the direct map, the authors learn the set of active constraints at optimality. This approach is efficient as the number of such active constraints is sparse over a range of operating conditions. In the context of AC OPF, the number of such active sets will not be small. However, we will follow a data-driven approach based on prioritizing constraints to learn and grouping constraints that are active together. Compared to the DC case, this will entail sparse classification of only subset of all constraints. In particular, we use machine learning on historical data to optimally learn groups of system constraints that enable fast computations of the optimal power flow problem for different system uncertainties.

We demonstrate the computational improvements of our approach through simulation on different test cases in the IEEE PES PGLib-OPF benchmark library.

## **Teagan Nakamoto**

Program: GRA/Post Masters  
School: Brigham Young University  
Group: Q-6  
Mentor: Nathaniel Sanchez

Category: Engineering  
Type: Individual  
LA-UR: 19-26009

### **Simulation of Curved Flyers for Exploding Foil Initiators**

Exploding foil initiators (EFIs) function on the shock impact of a metal or plastic flyer that is nominally flat. In 2016, Wiley et al. produced x-ray images and 3D reconstructions of mid-action flyers that were shown to have measurable curvature. In this project, we use LANL's FLAG hydrocode to explore the shock response of materials to EFI flyers of varied curvature.

**ThienAn Nguyen**

Program: GRA/Post Masters

School: University of Florida

Group: NEN-5

Mentor: Russel Johns

Category: Engineering

Type: Individual

LA-UR: 19-26495

## **TRACE Modeling of Closed-Loop, Lead-Cooled Cartridges for Use in the Versatile Test Reactor**

TRACE is a thermal-hydraulics code aimed at modeling nuclear systems and other two-phase flow problems. In this case, a closed-loop lead-cooled test cartridge is modeled. This type of cartridge is to be one of many in the Versatile Test Reactor (VTR) and it is designed to house one or more test samples in addition to any other measurement apparatuses. The VTR itself is a sodium-cooled fast test reactor created with the main purpose of irradiating various materials in a harsh environment of fast spectrum neutrons and high temperatures.

TRACE is utilized to analyze liquid lead flow conditions for various flow areas and hydraulic diameters of the fuel region. These values are varied to represent specific configurations of the fuel pins and the surrounding cladding and cooling structure. Some examples are a 7-pin hexagonal cartridge and a 4-pin cylindrical configuration. These models are compared and supported by a similar array of numerical tests performed by STAR-CCM+ for steady state of normal operational condition. Additionally, any transient scenarios will be initialized and solved by TRACE. These time-dependent system characteristic predictions are of paramount in understanding of the VTR system design, which CFD code cannot economically provide due to computational restrictions.

## **Thomas Roberts**

Program: GRA/Post Masters

School: University of Utah

Group: E-13

Mentor: Scott Ouellette

Category: Engineering

Type: Individual

LA-UR: 19-26289

### **Dynamic Effects of Preload in Hyperelastic Foam Models**

Engineering analysts have a need to understand the effect that preload in closed-cell foams has on the dynamic response of a suspended mass. Currently, the effects of preload, or pre-compression, are considered to be negligible; however, any effect to the dynamic response could be detrimental to the involved system. The approximate cubic relationship between force and displacement of the material of interest poses an interesting problem in analyzing how the frequency response of the suspended mass changes with transitions from the cell wall bending to the more linear portion of the stiffness profile. A suite of studies utilizing finite element analysis and numerical simulations was used to perform a parametric study in order to generate a material meta-model that accurately describes the nonlinear system dynamics. Material properties such as density, porosity, and other hyper-elastic characteristics within the parameter space were varied in these simulations. A simple two-dimensional plane strain FE model including two sections of closed cell foam and one section of a solid mass was used to perform two tasks – implicitly determine stress states from pre-compression in the foam and explicitly solve for the system's dynamic response when subject to an initial velocity. These results were then verified using numerical simulations of the Duffing-like oscillator's second-order equation of motion. A single-element, plane strain model of the closed-cell foam was used in a cyclic fashion to generate data points for creating force-displacement curves that were fitted to create a functional model for the foam's stiffness. Time history signals of the oscillator's response to an initial velocity from both analysis methods were then transformed to the frequency domain where the parameter of interest was the fundamental frequency of the system. The fundamental frequency of the system was extracted from each set of data from the simulation suite. A sensitivity index for material model parameters was then formed based on the effect each parameter had on the frequency response of the system.

## **Athena Sagadevan**

Program: GRA/Post Masters  
School: Texas A&M University  
Group: NEN-2  
Mentor: Theresa Cutler

Category: Engineering  
Type: Individual  
LA-UR: 19-26498

### **Investigating Gamma Simulation Results for the SCRaP Experiment**

Benchmark experiments were performed in December 2016 using seventeen separate subcritical configurations of  $\alpha$ -phase plutonium sphere reflected by copper and polyethylene. These experiments took place at the Nevada National Security Site's National Criticality Experiments Research Center. To support the benchmark further, gamma simulations of the experiment will be performed using Monte Carlo N-Particle Transport Code and Gamma Detector Response and Analysis Software-Detector Response Function. The results from both codes will be compared and contrasted. In addition, simulations will be bettered to correctly capture the experimental conditions of the setup by comparing simulation and experimental data. Conclusions from this work will be used to bolster the benchmarking experiments that have been performed.

## **Andy Shen**

Program: UGS/Postbac

School: University of California, Los Angeles

Group: E-2

Mentor: Jeffrey Hyde

Category: Engineering

Type: Individual

LA-UR: 19-26891

### **Analyzing Hiring Needs for LANL's Plutonium Mission**

The Process Modeling and Analysis group (E-2) is performing an analysis on staffing and workforce trends based on the laboratory's goals for its plutonium pit production mission. For the past year, E-2 has been interviewing managers of various divisions and organizations that contribute to the pit production mission of the laboratory and collecting each group's required number of new hires and full time equivalents (FTEs), access requirements, and other supporting information for each pit production milestone. In addition, data is being gathered to assess the impact of the increased pit production on other missions at LANL. Once completed, the data from the interviews will be used to determine funding and infrastructure requirements for the lab. A detailed staffing analysis will be performed that incorporates the raw data obtained and attrition information to provide staffing information for the divisions included in the evaluation. Program managers can utilize the number of FTEs to distribute these employees amongst various projects and allocate funding for such projects, while Capital Projects and Human Resources assess how many individuals are hired in order to provide adequate office and parking spaces. The results are provided to various internal and external customers in order for them to determine how much infrastructure and funding are needed to accommodate this growing workforce. This analysis will help to ensure that LANL has the required employees and infrastructure needed for the laboratory to maintain consistency and meet its pit production milestones. Current results across all show a significant need for more employees lab-wide in order to support the plutonium mission.



## Kristin Smith

Program: GRA/Post Masters

School: Texas A&M

Group: NEN-2

Mentor: Rene Sanchez

Category: Engineering

Type: Individual

LA-UR: 19-26897

## **Benchmark Analysis of Component Critical Configuration of KRUSTY**

Kilowatt Reactor Using Stirling Technology (KRUSTY) is a prototype designed as a proof of concept for NASA's Kilopower program, which was funded in order to create a small reactor for various space applications, including providing power for a colony on Mars or the moon. The experimental campaign for the sixty component critical configurations of KRUSTY lasted from November 2017 to March 2018. KRUSTY was an annulus of HEU fuel reflected by beryllium oxide (BeO) and stainless steel (SS).

Of the sixty configurations created, five were chosen to be evaluated as benchmark cases. The configurations differed based upon the height of the BeO reflector rings, the axial reflector plug material, and the presence of an AmBe source.

The KRUSTY benchmark evaluated all sources of experimental uncertainty: measurement, mass, dimension, composition, and position. The evaluation of the uncertainties was completed by creating upper and lower perturbed cases for each uncertainty. The perturbed cases were simulated using MCNP6.2® with a total of one billion active histories for a Monte Carlo uncertainty of 0.00002 (2 pcm) for each case.

The effect of the uncertainty,  $\partial k_{\text{eff}}$ , was calculated via Eq. 1, where  $u_i$  is the standard uncertainty in the parameter being perturbed,  $\partial x_i$  is the value of the perturbation, and  $\Delta k_{\text{eff}}$  is the difference in the  $k_{\text{eff}}$  for the perturbed cases.

$$\partial k_{\text{eff}} = u_i / (\partial x_i) \Delta k_{\text{eff}} \quad (1)$$

This poster presents a summary of the uncertainties for all benchmark cases.

## **Joshua Tempelman**

Program: GRA/Post Masters  
School: Michigan State University  
Group: NSEC  
Mentor: Adam Wachtor

Category: Engineering  
Type: Individual  
LA-UR: 19-25875

### **Acoustic Monitoring for Defect Detection in Metal Powder-Bed Laser Sintering**

In-situ monitoring of additively manufactured (AM) parts has become a topic of increasing interest to the manufacturing community, because defects in AM parts are generated as the part is built. In this work, the use of acoustic measurements of metal powder-bed laser sintering processes were investigated as a detection tool for pore formation made during the sintering process. Post-build radiography images were used to locate pores, which are correlated with localized acoustic time series partitions (0.5-1.0 seconds). Ensemble empirical mode decomposition (EEMD), singular spectrum analysis (SSA), and statistical measures of the time series partitions were used to extract feature vectors which correlate to pore formation. Sequential feature selection revealed that measures associated with EEMD are most useful in classifying acoustic monitoring data accordingly. The reduced feature vectors were then used to train a support vector machine model to predict pore formation with up to 95% accuracy.

## **Cole Thompson**

Program: GRA/Post Masters  
School: University of Texas at Austin  
Group: PT-3  
Mentor: Brian O'Neil

Category: Engineering  
Type: Individual  
LA-UR: 19-26118

### **An In-line Neutron Coincidence Counter for Plutonium Mass Quantification**

Calorimetry is a time consuming nondestructive assay for plutonium mass quantification in both person hours and sample measurement. Decreasing the amount of time needed for mass quantification to similar levels of uncertainty through an alternative assay would increase the efficiency of plutonium purification operations. The Blister Neutron Coincidence Counter, BliNCC, which can be added to a glove box, reduces person hours and count time by reaching one percent relative standard error of counts in a few hours for samples of low mass and low Plutonium-240 content and less than five minutes for samples larger than 1000 grams of any Plutonium- 240content.

## **Amy Ticklenberg**

Program: GRA-Post Masters

School: University of St. Thomas, University of Minnesota

Group: E-1

Mentor: Ryan Holguin

Category: Engineering

Type: Individual

LA-UR: 19-26726

## **Characterization of Helium and Argon Supersonic Jets Entering Variable Pressure Experimental Chamber**

In this characterization study, supersonic helium and argon jets expanding freely into an experimental chamber at a range of pressure ratios are analyzed. The pressure ratios studied vary from 20:1 up to 2000:1 and are achieved by evacuating the chamber down to ~1 psia and injecting helium or argon from 6000 psig gas cylinders. The experimental setup involves a variety of diagnostic techniques including Schlieren imaging, hotwire anemometry, and an array of pressure sensors.

The Schlieren imaging uses a Z-type configuration with a green LED light source, two eight-inch mirrors, and a Photron model WX-50 mini high-speed camera. TSI's IFA-300 Constant Temperature Anemometer is used with thin-film hotwire probes. Pressure sensors in the setup include five PCB piezoelectric 113B22 high-frequency pressure transducers, an Omega PX613 pressure transducer, and a Stellar Technology ST350 pressure transducer. The high speed images reveal the Mach disk location and height, shock lines, and spread angle of the jet. Hotwire anemometry measures the jet velocity 4 in downstream of the nozzle along the jet centerline. The array of pressure sensors tracks the pressure along the flow system and captures the stagnation pressure at four points along the back wall of the chamber. This data shows details of how the jet fills the experimental chamber through entrainment, jet expansion, shock development, and turbulence development at each of the pressure ratios between the injected gas and the chamber air.

Synchronizing all of these measurement systems to capture the high-speed jet occurrence requires rapid data acquisition and precision triggering. This is achieved with a Stanford Research Systems model DG645 digital delay generator and a National Instruments cRIO-9047. The data collected from each test is correlated based on a dimensional analysis to gain a greater understanding of the transient jet behavior.

## **Annie Ung**

Program: GRA/Post Masters  
School: University of Texas at Austin  
Group: W-10  
Mentor: Jonathan Mace

Category: Engineering  
Type: Individual  
LA-UR: 19-26354

## **Quantification of Margin and Uncertainty for a Neutron Radiography Application**

Quantification of Margin and Uncertainty focuses on identification, characterization, and analysis of thresholds and associated margins for engineering systems under uncertainty. This is especially useful for complex systems where comprehensive experimental test data is not readily available. This methodology is practiced on a neutron radiography application to gain familiarity with the tool. A neutron radiography experiment and a radiation transport simulation will also be conducted. The results will then be evaluated to draw conclusions on the methodology, with the hope of extending it to other nuclear engineering applications.

## **Marshall Vaccaro**

Program: UGS/Postbac

School: Missouri University of Science and Technology

Group: ISR-4

Mentor: Jeremiah Rushton

Category: Engineering

Type: Individual

LA-UR: 19-26351

## **Radar Imaging of High Explosive Detonations Using an Ultrawide Bandwidth Antenna**

The imaging of high explosives using radar technology is met with challenges that require antennas with high bandwidth for accurate spatial resolution, high gain for adequate signal strength, and low cost due to the risk of damage to the antenna. Vivaldi antennas are an inexpensive tapered-slot antenna design that combines high gain and a frequency-independent bandwidth. Vivaldi antennas can be easily combined with metamaterials, which can be designed to shape various aspects of the antenna's radiation pattern and enhance gain in the end-fire direction. These antennas are also made by printing a conducting sheet onto a dielectric substrate, which makes them relatively low cost and easily reproducible. This presentation is for a novel design of a printed Vivaldi antenna with low side lobe levels and high gain across Ka band. The performance of the antenna is achieved with an epsilon near zero metamaterial to enhance directivity, and quarter-wave corrugations on the antenna in the end-fire direction to reduce side lobes and enhance gain.

**Julien Valdez**

Program: UGS/Postbac  
School: University of New Mexico  
Group: SSO-1  
Mentor: Scott Mcduffie

Category: Engineering  
Type: Individual  
LA-UR: 19-26795

**Mechanical Engineering**

My poster will be talking about the mechanical engineering field. It will consist of different topics such as what is a mechanical engineer, job duties, jobs and salary, what a masters and Ph. D does, and the pros and cons of becoming a mechanical engineer.

## **Mario Valles Montenegro**

Program: GRA/Post Masters  
School: University of Nevada Las Vegas  
Group: M-9  
Mentor: Forrest Svingala

Category: Engineering  
Type: Individual  
LA-UR: 19-26970

### **Gas-Gun Target for High-Temperature Plate Impact of Insensitive High Explosives (IHE)**

Gas-Gun Target for High-Temperature Plate Impact of Insensitive High Explosives (IHE) High explosives (HEs) are an essential component for munitions, non-nuclear weapons, and nuclear weapons; however, they carry a significant safety risk. Based on these motives, Department of Energy (DOE) and Department of Defense (DOD) scientists and engineers developed IHE [1]. These improved the safety and survivability of munitions, weapons, and personnel significantly, as well as reduced the risk of detonation by impact, heat, or shock. Nevertheless, new IHE still requires standard testing [see MIL-STD-2105 and LA-UR-15-29238], which comprises undesirable perilous and wasteful aspects, to be qualified as insensitive. Considering these factors, we tested an inert target and a setup design that alludes how a new- IHE-system will behave. The tested material had similar characteristics to the IHE to be tested, with a high-temperature range (204 °C), sufficient for IHE qualification testing (200-250 °C). The tested setup consisted of novel engineering design, employing metallic screws and heat- resistant-plastic springs; it allows the removal of all HE-compatible adhesives – which fail at high temperatures. Time and temperature were measured with thermocouples devices to observe the inert sample thermal gradient. Decisively, experimental results indicate, the new setup arrangement will be performed adequately for the new type IHE, and it will enable further IHE testing with similar characteristics. Thus, we report on this poster a nova forma of system evaluation that increases safety and efficiency.

Simpson, Randy. "Unraveling the Mystery of Detonation." High-Explosives Detonation Research, Lawrence Livermore National Labs, June 1999, [str.llnl.gov/str/Simpson99.html](http://str.llnl.gov/str/Simpson99.html). Science & Technology Review 1999



## **Eppie Velarde**

Program: UGS/Postbac  
School: New Mexico Tech  
Group: Q-18  
Mentor: Ernest Salazar

Category: Engineering  
Type: Individual  
LA-UR: 19-26862

### **Thermal Conditioning of Engineered Components**

Thermal conditioning is an integral part of engineered component testing. By altering the thermal state, this allows the engineer to understand how a component changes or 'reacts' to a wide range of temperatures. The coefficient of thermal expansion, or CTE is used to determine the rate at which a material expands as a function of temperature. CTE is used for design purposes to determine if failure by thermal stress may occur. Understanding the relative expansion/contraction characteristics of materials helps us in thermal conditioning of engineered components. Thermal conditioning of components also helps us to understand what kind of environments they will function as they are intended to.

**Kelley Verner**

Program: GRA/Post Masters

School: University of Idaho

Group: NEN-5

Mentor: Seung Jun Kim

Category: Engineering

Type: Individual

LA-UR: 19-26314

## **Production of Molybdenum-99 via Fissile Solution Reactor and Electron Beam Accelerator**

Molybdenum-99 is a medical isotope critical in numerous medical imaging techniques used today. However, Mo-99 is not used directly in the imaging applications. Its daughter product, technetium-99m (Tc-99m) is the actual isotope required. The 6-hour half of Tc-99m does not allow for transportation and use. This is why Mo-99 is produced instead; it has a half-life of 66 hours. While this is enough time to use the isotope, it does not allow for any stockpiling of the material and it must be produced as needed. The United States has no domestic supply of Mo-99 and must rely on outside entities for it, creating an economic and national security risk. Many methods for Mo-99 production exist; this work explores the unique idea of using a fissile solution reactor with a horizontal electron beam accelerator to produce the isotope of interest. A uranyl nitrate solution along with a depleted uranium target are used. When the electron beam interacts with the DU target bremsstrahlung gamma rays are produced and subsequently neutrons via photofission. These react in the fissile solution to cause a chain reaction. Mo-99 is one of many fission products of the (n,f) U235 reaction. The goal of this work is to maximize the Mo-99 yield from this reaction. Three conditions are considered to improve the yield modeled in MCNP; target geometry, target placement within the vessel, and additional materials in the vessel to increase neutron flux. Each condition will be modeled with MCNP, and using the F4 flux tally and F8 energy tally, the theoretical Mo-99 production will be calculated. In future work, the results will be coupled with computational fluid dynamics models to create an iterative process by which Mo-99 yield will be maximized with a more accurate model of the system's thermodynamics and fluid dynamics.

## **Do Vo**

Program: High School  
School: University of New Mexico  
Group: MPA-MAGLAB  
Mentor: Doan Nguyen

Category: Engineering  
Type: Individual  
LA-UR: 19-21533

## **Comprehensive Finite Element Modeling for Pulse MAGNET DESIGN Using COMSOL and Java**

Ultra-high field pulsed magnets must simultaneously satisfy a number of often competing electrical, electromagnetic, structural, thermal, and economic constraints. To produce the highest field possible, nondestructive pulsed magnets are designed to operate at the limits of mechanical strength, electrical carrying capacity of conductors and availability of power resources. In this presentation, we will introduce a coupled multi-engineering finite element method (FEM) implemented in COMSOL™ Multiphysics package for detailed and accurate calculations of the mechanical, thermal and electromagnetic performances in entire longitudinal cross-section of the pulsed magnet. These transient FEM simulations are performed for entire pulse length and take into account the temperature and magnetic field dependencies of electrical conductivity and mechanical properties of all the materials to provide better accuracy. Java Software and Application Programming Interface (API) feature of COMSOL were used to automate repetitive modeling steps to significantly reduce the necessary time to create FEM models for a pulsed magnet which may consists up to thousands of turns and insulation/reinforcement layers. Computational results for our signature 100T non-destructive pulsed magnet will be presented.

## **Jianchao Zhao**

Program: UGS/Postbac  
School: University of Louisville  
Group: C-CDE  
Mentor: Kwan-Soo Lee

Category: Engineering  
Type: Individual  
LA-UR: 19-25845

### **Silicate Sequestration for Water Treatment**

Water is extensively used in industry as a common cooling fluid, due to a number of advantages such as its high heat capacity and cost effectiveness [1]. However, its use inevitably leads to an undesirable side effect, scale formation, when supersaturation occurs, causing silicates to precipitate out of solution. Ground water in Los Alamos has an abnormally high silicate concentration at about 90 ppm, while the silicate solubility (which depends on water chemistry, temperature and other factors) is generally accepted to be approximately 150 ppm. Therefore, operators must maintain silica at an acceptable level to avoid silicate deposition. This requires operating cooling systems as very low cycles of concentration, resulting in a very inefficient use of water. To combat this issue, this work has proposed the use of a green polymer additive polyethylene glycol (PEG) for silica scale inhibition by increasing the silica solubility limit. It has been shown in the literature that the molecular weight and concentration of PEG has an effect on the level of silica scale inhibition [2-3]. This work investigates the use of four different molecular weights of PEG: 1000, 2000, 10000 and 20000 and determines the optimal concentration for each. The concentration of silicates in solution was quantified using a high range silica test with a Hach spectrophotometer. Significant enhancements in silica solubility were observed for several water sources across the laboratory. These results provide a foundation for eventually increasing the number of allowable cycles used in cooling systems across the laboratory.

[1] Ashdown, P., Ashworth, D. and Guthrie, W. (1999) Water, water, everywhere, Performance Chemicals Europe, November/December, 28-29.

[2] Preari M., and Demadis K.D. "The use of Environmentally-Friendly and "Green" Polyethylene Glycol Additives for Silica Scale Inhibition and Control in Industrial Water Flow Systems." Proceedings of the 13th International Conference of Environmental Science and Technology. Athens, Greece, 5-7 September 2013.

[3] Demadis, Konstantinos D., and Melina Preari. "'Green' scale inhibitors in water treatment processes: the case of silica scale inhibition." *Desalination and Water Treatment* 55.3 (2015): 749-755.

## **Natalie Aulwes**

Program: High School  
School: Los Alamos High School  
Group: E-6  
Mentor: Joseph Hashem

## **Adam Schmidt**

Program: UGS/Postbac  
School: New Mexico Institute of Mining and Technology  
Group: E-6  
Mentor: Joseph Hashem

Category: Engineering  
Type: Group  
LA-UR: 19-25940

## **Automating X-Ray Imaging of Radioactive Components with Robotics**

We have developed a robotically controlled non-destructive testing imaging system for x-ray radiography and computed tomography. In this effort, a robotic manipulator is implemented as the motion control system for x-ray imaging tasks. This system incorporates a collaborative six-axis robot, a 150 keV micro-focus x-ray source, and a 127-micron digital detector. The robotic positioning arm is programmable and allows imaging in multiple configurations including planar, cylindrical, as well as other user-defined geometries that provide enhanced automated capability. To illustrate the advantages of using a robot with x-ray imaging, mock liner welds (heat sources) were characterized using x-ray radiography. The robot has to shake the part in order for the powder to settle at the bottom before imaging, which is required in order to take measurements on the part's weld. Flexible automation with non-destructive imaging reduces dosage since the human operator no longer has to handle the parts.

## **Colin Brennan**

Program: UGS/Postbac  
School: University of Texas at Austin  
Group: W-10  
Mentor: Jonathan Mace

## **Matthew Webb**

Program: GRA/Post Masters  
School: The University of Texas at Austin  
Group: W-10  
Mentor: Laura Cartelli

Category: Engineering  
Type: Group  
LA-UR: 19-26013

## **Electrostatic Discharge Experiments for Validation of the Plasma Kinetic Model**

Colorado School of Mines (CSM) in partnership with Los Alamos National Laboratory (LANL) has developed a Plasma Kinetic Model to characterize energy deposition from an electrically charged surface to a victim load during threshold sparks. An experimental capacitor system has been developed at LANL to induce and measure threshold sparks for comparison to simulated events. This project explores the data from several variations of the spherical capacitor system and compares it to the Plasma Kinetic Model and previous efforts to simulate threshold sparks.

**Adam Collins**

Program: UGS/Postbac  
School: Worcester Polytechnic Institute  
Group: WI-PO/ALDCP  
Mentor: Karen Borovina

**Matney Juntunen**

Program: UGS/Postbac  
School: Montana State University  
Group: ES-UI/ALDCP  
Mentor: Genna Waldvogel

**Julianne Sanscartier**

Program: UGS/Postbac  
School: Carnegie Mellon University  
Group: ALDCP  
Mentor: Matt Foster

**Troy Sims**

Program: UGS/Postbac  
School: New Mexico Institute of Mining and Technology  
Group: ALDCP  
Mentor: Paul Stevenson/Steve Renfro

**Jake Torrez**

Program: UGS/Postbac  
School: Baylor University  
Group: ALDCP  
Mentor: Matt Foster

Category: Engineering  
Type: Group  
LA-UR: 19-25681

## **Smart Lab Renovation for TA-03-1420**

While the Center for Integrated Nanotechnologies (CINT) succeeds in achieving a mission focused on the world-leading technological innovation of nanostructured materials, its 21st century building fails to reach its highest potential for efficient energy use. Recent strides for energy conservation, as a result, leave CINT falling behind both the Department of Energy and Los Alamos National Laboratory's critical energy-saving goals. Our solution utilizes UC Irvine's Smart Lab design--a carbon abatement and energy efficient strategy. As the Smart Lab team for the summer of 2019, we developed a new design for CINT which addresses the seven key elements of a Smart lab that need adjustment or are completely missing: digital control systems, demand-based ventilation, low power-density demand based lighting, exhaust fan discharge velocity optimization, pressure drop optimization, fume hood flow optimization, and commissioning with automated cross-platform fault detection. At its current state, CINT not only lacks efficient lighting techniques, but the HVAC design also functions twenty-four hours a day without the correct set-up to fully utilize building automation and optimization. A renovation and project plan was delivered to Capital Projects (ALDCP) during the first week of August, 2019. Efficiency goals throughout the design process were to meet the FEMP required 30% better than the ASHRAE 90.1 energy baseline. This was accomplished through our recommendation of elements for Smart Lab implementation regarding the programmatic aspects of CINT. In offering a complete design package of updated CAD drawings, line diagrams, schedules, and a life-cycle cost analysis, this project will upgrade CINT to a facility that lives within its own mission.



**Jorge Garcia**

Program: GRA/Post Masters  
School: New Mexico State University  
Group: ADPO  
Mentor: Jen Bohon

**Christopher O'Neal**

Program: UGS/Postbac  
School: Texas Tech University  
Group: ADPO  
Mentor: Jen Bohon

**Adrianna Ortega**

Program: UGS/Postbac  
School: University of Denver  
Group: ADPO  
Mentor: Cris Barnes

Category: Engineering  
Type: Group  
LA-UR: 19-25938

## **Conceptual Design for a Portable Additive Manufacturing In-Situ Diagnostic End-Station**

While the field of additive manufacturing (AM) has potential for transforming the manufacturing industry, full control of AM processes has not been yet achieved. Unexpected results that affect the overall quality and performance of parts, such as splattering, porosity, or residual strain, are not completely understood and present a recurring challenge in the field. These subtle but impactful defects occur at the materials mesoscale, which cannot be observed in the visible spectrum. These micron-sized errors can be resolved both spatially and temporally through the use of hard x-rays, generated from synchrotrons or free electron laser facilities. In order to meet the demands of current and future research endeavors, we aim to design a portable and adaptable system capable of hosting different AM experiments at various x-ray beamlines to characterize the dynamics which materials undergo in AM processes. We will show a conceptual design for such an experimental end-station. It will consist of a dual-chamber system that will allow the capability of controlling environment parameters, such as temperature and pressure, as desired. Through the use of adjustable collimator settings, the incoming x-ray beam can be manipulated to accommodate a desired detection scheme. This would enable data collection for multiple in situ diagnostic techniques. Optimization of experimental parameters can be potentially achieved through the use of machine learning-based systems. This automation of the scientific process would enable improved results in a shorter time period than those of traditional experiments. This end-station would enable accurate characterization of the AM processes, revolutionizing applications that are of interest to both industry and national security.

## **Sabina Gulick**

Program: UGS/Postbac  
School: New Mexico Tech University  
Group: EES-14  
Mentor: Manvendra Dubey

## **Jaimy Karacaoglu**

Program: UGS/Postbac  
School: New Mexico Institute of Mining and Technology  
Group: EES-14  
Mentor: Manvendra Dubey

Category: Engineering  
Type: Group  
LA-UR: 19-26995

## **Biomass Combustion Aerosols and Their Surrogates: Characterizing Key Optical Properties Using Advanced Techniques**

Smoke emitted from wildland fire has a significant and increasing impact on air quality in New Mexico. Wildfires and prescribed fires contribute atmospheric particulate matter and gas-phase pollutants impacting visibility, human and ecosystem health, and regional climate. By analyzing wildfire measurements, laboratory burns, and synthetic carbon dye data, we are able to quantify and attribute characteristics to fuel types, combustion temperature and environmental parameters such as relative humidity. Measurements include light scattering, absorption, extinction, water uptake ( $f(RH)$ ) at a range of humidity from 20% to 90%, black carbon mass, and single scattering albedo (SSA). Custom humidity-controlled measurement systems include dual nephelometer and humidity-controlled cavity attenuated phase shift monitor (CAPS), both developed in-house. Calibration aerosols including ammonium sulfate and nigrosin validated instrument behavior. Laboratory burn experiments showed a pronounced influence of combustion temperature alternately producing collapsing sooty aggregates (low temperature glowing combustion) or a hydrophilic aerosol (high temperature flaming combustion). On 21 June 2019, the Woodbury Fire east of Phoenix, Arizona produced strong smoke impacts in Los Alamos, New Mexico. Key ambient results include the analysis of the Woodbury Fire plume, which indicated it is aged for about half a day before arriving in Los Alamos, NM, had little humidity dependence, and has an SSA of 1, indicating that it is a mostly scattering plume composed of volatilized organic compounds with very little inorganics. These parameters help determine whether aerosol particles cause a net cooling or warming impact on climate.

## **Leah Lujan**

Program: UGS/Postbac  
School: New Mexico State University  
Group: Q-17  
Mentor: Michael Steinzig

## **Hayden Randall**

Program: UGS/Postbac  
School: New Mexico State University  
Group: Q-17  
Mentor: Mike Steinzig

Category: Engineering  
Type: Group  
LA-UR: 19-26692

## **Pressure Vessel Analysis**

The objective of this experiment is to determine a priori, the internal pressure of a vessel, by making strain measurements on the outside of the vessel. To demonstrate this ability, the method being focused on is changing the temperature of the liquid in the vessel and measuring the resulting change in strain on the outer surface of the vessel. To demonstrate the technique, a full soda can is used to represent a pressurized cylindrical vessel. The CO<sub>2</sub> pressure from the soda results in hoop strain around the circumference as well as longitudinal strain along the length. The change in pressure that occurs during a change in temperature is a result of the changing solubility of CO<sub>2</sub> in the liquid soda. This relationship is known, and thus the expected change in pressure for a given change in temperature can be calculated for the closed volume of the soda can.

The theory to determine if the actual pressure can be determined using this technique is still being developed. First, the ability to correlate change in pressure with change in strain will be demonstrated. In order to measure strain, strain gauges are installed and connected to a Model P3 Strain Indicator and Recorder by Vishay. The temperature of the soda can will be measured and controlled changes in temperature will be introduced, with plots of the change in pressure as a function of temperature produced for the soda can. As a final step, the can is opened and the curve extended to the known zero pressure. In this experiment, it is possible that the initial state of pressure can be determined a priori because the solubility curve is non-linear, thus allowing a particular state to be identified by measuring only pressure-induced changes in the strain.

## **Renan Rojas-Gomez**

Program: GRA/Post Masters  
School: University of Illinois at Urbana Champaign  
Group: NSEC  
Mentor: Youzuo Lin

## **Jihyun Yang**

Program: GRA/Post Masters  
School: Colorado School of Mines  
Group: NSEC  
Mentor: Youzuo Lin

Category: Engineering  
Type: Group  
LA-UR: 19-26678

# **Data-Driven FWI Methods for Seismic Imaging: Generalization and Robustness Study**

Recently developed data-driven Acoustic and Elastic Waveform Inversion (AEWI) techniques for geophysical data analysis have shown outstanding performance, surpassing conventional model-driven methods in both accuracy and computational efficiency. However, despite their promising results, practical application of such data-driven methods is severely limited by the lack of real data available to train them, and how well these characterize the seismic scenarios of interest. Furthermore, State-of-the-Art data-driven techniques, which include well-established Encoding-Decoding and Generative Adversarial Networks, are typically trained using simplified synthetic datasets under ideal conditions i.e. without any noise component, which dismisses the diversity of velocity models and source-receiver geometries from practical scenarios.

Based on this, an in-depth analysis of the generalization and robustness properties of multiple State-of-the-Art data-driven AEWI methods under complex synthetic scenarios is presented. The performance is evaluated using a novel CO<sub>2</sub> leakage dataset, generalization is evaluated by measuring the cross-domain knowledge of the parameters obtained by learning over a synthetic dataset with abundant training pairs and evaluating the regression accuracy over samples with distinct distributions. Similarly, robustness is evaluated by measuring the prediction accuracy under the presence of physically coherent distortions such as missing sources, non-uniform receiver coverage, and coherent noise. Finally, an extension of the well-established Fully Convolutional Neural Network Architecture (FCN) is developed in order to improve the robustness and transferability of recent machine learning AEWI approaches. Quantitative results based on classic metrics such as MSE, MAE and MSSIM, as well as reconstructed velocity maps.

# **HEALTH & SAFETY**

## **Michelle Barkley**

Program: UGS/Postbac  
School: University of Texas-San Antonio  
Group: EPC-ES  
Mentor: Terence Foecke

Category: Health & Safety  
Type: Individual  
LA-UR: 19-26895

### **What is a hazardous chemical? Refining how chemicals are managed at LANL based on human health risk.**

What is a chemical? There are many interpretations on the definition of a “chemical,” but based on the definition adopted by our regulators, everything is a chemical. Our current chemical inventory system, “ChemDB,” provides a database that holds information on all materials classified as a chemical by these regulators. This database keeps the laboratory in compliance, but doesn’t efficiently utilize the influx of information within the system to optimize chemical safety and transparency here at LANL. Our current system holds all materials in the chemical inventory to the same standard, regardless of the differing physical and health hazards associated with each chemical. This study researches a new adopted algorithm for identifying what exactly a chemical is at Los Alamos, and what exactly we should care about. This will allow a thorough consolidation of our current inventory to set a scope on which chemicals require the most accountability, tracking, and hazard transparency, while developing a way to identify non-hazardous commercial chemicals that pose minimal risk to employee safety here at Los Alamos. This research will calculate the total cost for the current chemical management process and identify how this new system will minimize cost and inventory data while maximizing safety.

## **Gabrielle Broadous**

Program: UGS/Postbac  
School: University of New Mexico  
Group: RP - SVS  
Mentor: Thomas Mclean

Category: Health & Safety  
Type: Individual  
LA-UR: 19-26032

### **Electronic Personal Dosimeter Performance as Function of Placement on a Realistic Human Torso**

Electronic Personnel Dosimeters (EPDs) measure, display, and record in real time the dose an individual may receive while working in a radioactive environment. The EPD should ideally be worn at the center of the sternum; however, it is often seen placed over the lungs, on shirt pockets, or even on the collar. The goal of this project is to determine how well EPDs measure dose as a function of placement and incident angle on a realistic human torso. The performance of the following three models of EPDs was tested in gamma, beta, and neutron reference fields based on radiological performance tests outlined in ANSI N42.20-2003 (American National Standard Performance Criteria for Active Personnel Radiation Monitors) and IEC 61256:2010 (Radiation protection instrumentation – measurement of personal dose equivalent radiations – direct reading personal dose equivalent meters):

- Mirion DMC 3000 EPD (beta and gamma fields)
- Thermo-Fisher Scientific TruDose EPD (beta and gamma fields)
- Thermo-Scientific EPD-N2 (neutron, beta, and gamma fields)



## **Kylie Gallegos**

Program: UGS/Postbac  
School: New Mexico State University  
Group: EPC-ES  
Mentor: Shannon Gaukler

Category: Health & Safety  
Type: Individual  
LA-UR: 19-26263

### **Benthic Macroinvertebrate Community Assemblages and Population Metrics from Ephemeral Streams on the Pajarito Plateau**

Climate change is continuously altering streams across the globe, making water quality monitoring more difficult. These changes in our ecosystem make finding effective methods of monitoring natural water sources critical. During 2017 and 2018, the Environmental Stewardship Group at Los Alamos National Laboratory collected benthic macroinvertebrates from dry and wet transects within ephemeral streams and compared population metrics and community assemblages between the two sample types. Benthic macroinvertebrates were collected via kick net when water was present and by a dry sediment grab when water was absent. Dry sediments were then inundated with water and benthic macroinvertebrates were collected after two weeks. Benthic macroinvertebrates were found in 42 of 46 samples collected. Diversity and the Hilsenhoff Biotic Index between dry and wet sample types showed no significant differences ( $p > 0.05$ ). However, abundance and species richness differed between sample types ( $p < 0.05$ ). The variability and community composition of benthic macroinvertebrates differed between sample types ( $p < 0.05$ ). Benthic macroinvertebrates collected from dry samples showed overall lower abundance and species richness when compared to samples collected from water; this difference is likely caused by the absence of water rather than to pollution or disturbance. Though investigating benthic macroinvertebrates from dry transects within ephemeral streams can lend information to general health of a stream they are not recommended as an accurate method of monitoring water sources. Monitoring benthic macroinvertebrates within water in ephemeral streams is more informative in regards to examining water quality.

## **Maeve Kelly**

Program: UGS/Postbac  
School: Colorado State University  
Group: RP-PROG  
Mentor: Jenelle Mann

Category: Health & Safety  
Type: Individual  
LA-UR: 19-26608

### **Comparison of MCNP Variance Reduction Techniques for Linear Accelerators**

Modelling of radiation shielding and dosimetry, as is performed by the Radiological Engineering group, is often performed using Monte Carlo methods with radiation transport codes such as Monte Carlo N-Particle (MCNP) Transport Code. This method is known for producing accurate results, but it can also be very time-consuming. Long computational run times can be reduced without sacrificing accuracy of results through the implementation of variance reduction techniques. Use of these techniques was assessed through modelling a 6MV linear accelerator, based upon the Varian Linatron K15 geometry. This accelerator operates by colliding monodirectional electrons in a vacuum striking a tungsten target, producing a field of photons via bremsstrahlung. The following MCNP calculation results were examined: the photon field produced, the beam dose at varying positions, and the leakage dose (to the side of the accelerator). Variance reduction techniques assessed include truncation techniques (phase space, energy cut offs, removal of knock-on electrons), modified sampling techniques (bremsstrahlung biasing), population control techniques (Russian roulette of low-energy particles), and partially deterministic techniques (forced collisions). Dose beam geometry and energy spectra were examined to investigate the effects of variance reduction techniques upon the MCNP calculation results. The comparisons include exploration of results in the context of a new feature to MCNP, utilizing unstructured mesh produced through the Atilla4MC software.

## **Francesca Pacheco**

Program: GRA/Post Masters  
School: University of New Mexico  
Group: TA-55-RLW  
Mentor: Sylvie Adam

Category: Health & Safety  
Type: Individual  
LA-UR: 19-26577

### **Portable Office Lighting and Eye Strain**

Eye strain is a multifactorial health issue that can interfere with an employee's performance. Over the past two years, the TA-55 Ergonomic Health and Safety professionals noticed an increase in reports of eyestrain, particularly employees in portable office trailers. 27% of the employees who received an office ergonomic evaluation reported eye strain symptoms (e.g., dry eyes, headache, blurred/double vision, and difficulty concentrating). According to Illuminating Engineering Society, the recommended light level for an office space is between 300- 500 lux. To investigate a possible connection between light level and employee eye strain in portable office trailer spaces, a survey was conducted. A combination of quantitative and qualitative data were collected for 116 employees. Each survey took approximately 4 minutes to complete and consisted of two questions and three light measurements. Although results from this survey, comparing eye strain and light level, proved to be statistically insignificant, our data shows that 59% of the population surveyed still experiences eyestrain regardless of ambient workstation light level. Further investigation would benefit the health and wellness of LANL personnel whose main offices are contained in portable buildings.

# **INFORMATION TECHNOLOGY**

## **David Butts**

Program: GRA-Post Masters  
School: Michigan State University  
Group: A-1  
Mentor: James Cooley

Category: Information Technology  
Type: Individual  
LA-UR: 19-26561

### **Using TRANSIMS for Evacuation Planning**

Evacuations of cities are necessary during emergency events like hurricanes and forest fires, but can be hard to prepare for due to the impracticability of evacuating a city during a non-emergency and the unpredictability of such events. Simulation can help bridge this gap by allowing for multiple scenarios and response plans to be tested for a city with very little cost. Transportation Analysis and Simulation System (TRANSIMS) is an open source, agent based traffic microsimulator that allows for detailed simulations of city traffic. In this project we use TRANSIMS to explore forest fire evacuation strategies for Los Alamos County. The strategies we are testing include simultaneous and staged evacuations, as well as the effects of opening back roads. We run a simulation by creating a synthetic road network with daily traffic and then adding evacuees to the network in a way that is consistent with one of the evacuation plans. The simulation allows us to see where congested roadways are and time how long an evacuation will take. This information can then be used to create better evacuation strategies.

**Jesse Ibarra**

Program: GRA/Post Masters  
School: New Mexico Highlands University  
Group: P-21  
Mentor: Aik-Siong Koh

Category: Information Technology  
Type: Individual Poster  
LA-UR: 19-26228

## **Combining the Most Desirable Object Oriented Programming Features**

Smalltalk is an object-oriented language that provides many useful capabilities that many programming languages don't offer. The use of Smalltalk's live programming capabilities allows the programmer to inspect and modify programming code in run time or while the program is running. Smalltalks and Smalltalks IDE's run in image based environments which allow the programmer to save their image at any point in execution and resume at the very state were they left off. Other programming languages such as C and Python lack these powerful and dynamic features. Although, Smalltalk's package development has decreased over the years, development for languages such as Python continue to vastly increase. Both Python and Smalltalk are dynamically typed OOP languages. The desirable features of Python are even better implemented in Smalltalk because Smalltalk is pure OOP: Everything is an object. Every operation is due to message passing. This purity permits live coding and debugging. Objects persist continually even after the image is shut down and restarted. Utilizing Python's deep learning, image processing and highly optimized libraries such as Numpy and Scipy in the back-end, while taking advantage of Smalltalks powerful programming abilities we will be able to increase programming productivity and create an influential tool.

## **Benjamin Kosko**

Program: UGS/Postbac  
School: University of Pennsylvania  
Group: XIT-DO  
Mentor: Kimberly Vigil

Category: Information Technology  
Type: Individual  
LA-UR: 19-26500

### **The Standard Occurrence and Remediation of System Vulnerabilities on High Security Networks**

Networks which require a high level of security maintenance often pose unique challenges to system administrators who seek to proactively anticipate and resolve system vulnerabilities. Large meta-studies of systems allow administrators to better predict and resolve vulnerabilities before they develop into larger threats. Pre-patch system analysis is a key component of such pro-active action and lays at the heart of efficient and secure network upkeep. Vulnerabilities arising out of Adobe Acrobat and Nessus, two widely used software applications, led to large amounts of potential system security breaches such as remote code execution or sensitive information disclosure. Analyzing relevant system data before and after such laboratory wide software patches provide insight into the effectiveness and necessity of such proactive action. Factors such as operating system, type of computer and the level of security risk are all taken into account when developing solutions to potential vulnerabilities and predicting future occurrences.

An Adobe Acrobat patch, pushed on 2/24/2019, affected 954 system throughout the laboratory. Before it was pushed, administrators both tested the patch on select systems and coordinated with the System Center Configuration Manager (SCCM) on potential fixes. When the patch was finally deployed the amount of affected systems was down to 153 (an 84% decrease). In March 2018, a glitch within the Nessus agent affected 11,065 systems. Before these vulnerabilities become system blockers a combination of collaboration with SCCM, who pushed a script to clean non-OS systems, and self-help emails brought the number of affected system down to 5624 (a 51% decrease).

The Acrobat and Nessus represent two distinct vulnerability origins and also affect a wide range of systems. Thus, the methods used, and the corresponding results produced, can be reasonably extrapolated to similar software and scanning agents.

## **Joseph Rabaut**

Program: UGS/Postbac  
School: Michigan Technological University  
Group: NIE-IS  
Mentor: Angela Valdez

Category: Information Technology  
Type: Individual  
LA-UR: 19-27062

### **Database Compliance Analysis**

NIE-IS uses Puppet to manage all their virtual machines (VMs) to make sure all maintain compliance with all the necessary updates and configuration settings deemed necessary. If one of these settings were to change it could result in data being lost or even a system being compromised. To help prevent this a system was developed to take weekly summaries of the reports Puppet makes. These summaries would go through a week's worth of reports to help show the necessary individuals when a corrective change was applied to a VM, why this changed happened, when it happened, and allow for a member of NIE to take a closer look to make sure nothing bad is happening.



## **Alex Vargas**

Program: UGS/Postbac  
School: Northern New Mexico College  
Group: ISR-3  
Mentor: Joseph Fresquez

Category: Information Technology  
Type: Individual  
LA-UR: 19-26764

### **An Alternate Hyper-converged Infrastructure?**

Traditionally Los Alamos National Laboratory has large implementations of Nutanix based Hyper-Converged Infrastructure (HCI). When working with HCI environments it offers a software- defined data center approach. This approach allows for added benefits that aren't regularly available with some of the current data centers that are based on semi-converged infrastructures. The data center being software-defined allows for better management and monitoring of systems while removing some of the possible man- made errors that can be made with the traditional data center. Troubleshooting the systems also becomes easier because everything is available from one software interface, whereas traditional data centers have multiple interfaces that need to be checked when troubleshooting. HCI has better scalability, when adding more nodes/chassis to the system you just need to connect them to the current HCI infrastructure and can finish the basic configuration through the management interface without having to go to any extra lengths as one might have to with current semi-converged data centers. HCI bridges the gap between having an cluster for storage and a cluster for compute. It allows you to converge all of the infrastructure requirements into one package. This convenience and scalability comes at a cost. Nutanix equipment is priced on the higher end. With this proof of concept. I will dive into an alternative HCI solution from an alternative vendor NetApp. To see if it stands up to the competition for being a only fraction of the cost and having similar specifications.

**Carlos Castellano**

Program: GRA/ Post Masters  
School: University of New Mexico  
Group: XIT-CSS  
Mentor: Sharon Dermer

**Valerie Duran**

Program: GRA/Post Masters  
School: Colorado State University  
Group: XIT-CSS  
Mentor: Melissa Ortiz

**Lauren Quintana**

Program: GRA/Post Masters  
School: Colorado State University  
Group: XIT-CSS  
Mentor: Melissa Ortiz

**Joselin Rascon**

Program: UGS/Postbac  
School: Northern New Mexico College  
Group: XIT-CSS  
Mentor: Jenelle Montoya

Category: Information Technology  
Type: Group  
LA-UR: 19-27035

## **Deploying LINUX Virtual Desktops Utilizing Zero and Thin Clients**

Microsoft Windows has been the dominant Operating System (OS) for Desktops in the Virtual Desktop Infrastructure (VDI) realm for years. However, we can't forget about a VDI solution for the Linux Desktop. At Los Alamos National Laboratory (LANL) XIT-CSS has been utilizing the Oracle Sun Ray as a thin client solution for the past decade. Back in 2014, when Oracle announced the discontinuation of the Sun Ray, our organization began looking for an alternative solution. The goal was to find a product that would allow us to have a smaller footprint in the data center but still provide a great user experience. We are currently moving to Linux VDI and utilizing our Hyperconvergence Nutanix Cluster.

Our team tested several cutting edge Zero and Thin Clients, PCoIP, Cloud Access Software and Blast protocol in hopes to find a solution that would give the end user a high performance, ultra-secure remoting and endpoint architecture. Our hopes were to have a solution where data stays secure and never leaves the Virtual Environment but also supports NVIDIA GPU's for high-end graphical displays.

This project entails a replacement for the Oracle Sun Ray leveraging various industry leading technologies such as; VmWare eSXi, vCenter, VmWare Enterprise Plus, Teradici PCoIP and RedHatEnterprise Linux with a Dell Wyse Zero Client.

# **MATERIALS SCIENCES**

## **Anisa Baines**

Program: UGS/Postbac  
School: Howard University  
Group: MPA-CINT  
Mentor: Millicent Firestone

Category: Materials Science  
Type: Individual  
LA-UR: 19-26915

### **Encapsulating Proteins in 3D Printed Artificial Biomembranes**

The organization and stabilization of biomolecules (e.g., proteins) offers significant opportunities for heterogeneous biocatalysis the fabrication of functional biomolecular materials. In this work we describe the stable reconstitution of a heme protein, horse heart Cytochrome c (Cyt. c) within 3D printed crosslinked chemical hydrogels. The crosslinked hydrogel is a biomembrane mimetic material that is prepared from a multicomponent amphiphilic mixture self-assembled in a KPi buffer (i.e., complex fluid). The complex fluid is composed of saturated phospholipids, 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC); a crosslinkable macro- monomer, triblock copolymer diacrylated PEO-PPO-PEO (F98); a water-soluble PEGDA700, and a co-surfactant, lauryl dimethylamine oxide (LDAO) dispersed in KPi. Small-angle x-ray scattering confirms the complex fluids adopts a multilamellar structure with the amphiphiles organized into a biomembrane mimetic architecture. Cyt. c, chosen as a model enzyme for its optical signatures that allow monitoring of integrity, is doped into the complex fluid and then stabilized within the aqueous domains of the visible-light initiated crosslinked complex fluid through the use of TEAO and Eosin Y photoinitiator system. Visible polymerization occurred approximately within 3 hours of constant ambient light exposure at room temperature. Further demonstrated the bulk visible light polymerization approach is readily adapted to visible light 3D printing using a digital light processing (DLP). The integrity of the cyt c is monitored by UV-Vis spectroscopy. ATF/FTIR spectroscopy was performed to verify successful crosslinking. The nanostructure of the builds was determined by small angle x-ray scattering (SAXS). In summary, a self-assembled complex fluid encapsulating cyt c was created and 3D printed in order to better understand protein polymer interactions. This work lays the foundation for the facile production of hierarchically ordered functional bionanomaterials.

## **Christopher Bond**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: SIGMA-2

Mentor: Joseph Wermer

Category: Materials Science

Type: Individual

LA-UR: 19-26530

## **Synthesis of Monolithic Yttrium Dihydride for Solid Nuclear Reactor Moderator**

Yttrium dihydride is being considered as a moderator for a small, all-solid, maintenance-free nuclear reactor. A reactor of this type is envisioned which would operate in a variety of conditions including outer space where the presence liquid coolants or liquid moderators is impractical. The reactor design being pursued will operate in the range of 500-700°C under normal conditions and up to 900°C under off-normal conditions. Yttrium hydride has an advantage for such a design because it has a high hydrogen density (up to .0909 g/cc) and a very low hydrogen dissociation pressure under the proposed normal and off-normal operating conditions.

Samples of yttrium dihydride were prepared by very slow hydriding of cast yttrium metal at a temperature of 800-850°C. A typical preparation would take about 5-7 days to complete. These conditions were necessary to prevent cracking of the material due to rapid expansion of the metal lattice caused by the reaction with hydrogen. The final product had a density approximately 12% lower than yttrium metal starting material. This poster will detail the synthesis process and characterization of the yttrium dihydride product. The poster will also describe future irradiation tests with these samples which will be performed in order to qualify yttrium dihydride as a nuclear reactor moderator.

**Jack Brett**

Program: GRA/Post Masters

School: University of Oregon

Group: MST-7

Mentor: Michael Blair

Category: Materials Science

Type: Individual

LA-UR: 19-26230

## **Investigating the X-ray Irradiated Degradation of PMMA through FTIR and 2D Correlation Spectroscopy Analysis**

Two-Dimensional Correlation Spectroscopy (2D-COS) has been seen to identify accelerated conditions in a material, which could greatly aid in polymer aging studies. 2D-COS is performed by exposing a sample to variable amounts of a time-dependent external perturbation and spectroscopically measuring material change. The validation of this technique could save valuable time and resources which can be lost through aging studies. In this study, the degradation of poly(methyl methacrylate) is investigated using Fourier-transformed infrared (FTIR) spectroscopy and 2D-COS and evidence of change in the material due to x-ray radiation dose was seen and characterized through 2D-COS.

## **Zachary Brounstein**

Program: GRA/Post Masters  
School: University of New Mexico  
Group: C-CDE  
Mentor: Andrea Labouriau

Category: Materials Science  
Type: Individual  
LA-UR: 19-25396

### **Developing Advanced Manufactured Composite Polymer Filaments for Extreme Environments**

Extreme environments producing elevated temperatures, chemical species, mechanical stress, and ionizing radiation are of serious concern in industries relying on either materials retaining their inherent properties throughout a process or on materials protecting its product's consumers and instrumentation from such aggressive conditions. In the current aerospace, defense, and nuclear industries, commercial products are used as protective barriers, but there are circumstances when these are less than ideal at providing optimal shielding against extreme settings, especially neutrons and gamma rays. As innovations to aerospace, defense, and nuclear technologies progresses, developing new engineering materials and composites for temperature, chemical, mechanical, and radiation shielding grows in importance.

In the present work, we used an advanced manufacturing (AM) technique known as Fused Filament Fabrication (FFF) to create novel feedstock composite materials for 3D printing. FFF is a layered AM process whereby thermoplastic filaments are heated up to their melting point and extruded into cross-sections of the end product.

Difficulties in creating composite filaments for FFF arise from fabricating a homogenous wire that has uniform thickness and a smooth surface. If a filament does not have these initial properties, then either the FFF process will not work or the end product will not be as desired. Creating a homogenous wire proves more difficult when different base and filler materials are used in the fabrication process, however, this can be solved if the different materials are combined in a liquid solution. Creating a wire of uniform thickness relies heavily on the extrusion process, whereby the temperature and extrusion speed are controlled.

In this study, homogenous composite filaments were prepared for AM from a variety of polymer bases and incorporated a high weight percent loading of metal fillers. Thermal, mechanical, chemical, and radiative properties were evaluated to determine the efficacy of this AM feedstock material fabrication process.



## **Zachery Brown**

Program: High School  
School: Los Alamos High School  
Group: P-27  
Mentor: Melvin Borrego

Category: Materials Science  
Type: Individual  
LA-UR: 19-25780

### **Vacuum Furnace with Oil Quenching Abilities**

We present the design of an oil quenching vacuum furnace on a laboratory scale replicating the commercial scale heat treatment capabilities of the SIGMA complex, in particular for uranium containing samples. Replication of the heat treatment capabilities will eliminate the need for transport of radioactive samples across public roads thus minimizing the time between repetitive in-situ neutron diffraction experiments carried out at the Lujan Center. The minimized time enables rapid successive cycles of in-situ deformation and heat treatments and optimizes the utilization of the neutron beam time. By using this vacuum furnace, we can better understand the effect of heat treating on the microstructure of the material to aid in future advanced manufacturing processes.

## **Andrew Cardin**

Program: GRA/Post Masters

School: Duke University

Group: MPA-CINT

Mentor: Abul Azad

Category: Materials Science

Type: Individual

LA-UR: 19-26989

### **Agile Metasurfaces for Beam Manipulation**

Communications technology continues to advance fostering a demand for systems with reduced size weight and power (SWaP) for the manipulation of signals - modulation, encoding, steering, and focusing. Satellite technologies provide a salient example of this demand, with new 'small sat' and 'cube sat' technologies being developed and deployed. For maximum efficiency, such satellites require lightweight, flat reflectors to manipulate incoming and outgoing signals. Metasurfaces offer a robust and customizable platform to address this technological need, with their ability to be tailored to a desired function at a subwavelength scale. To date static versions of flat reflecting optics have been demonstrated with metasurfaces, and in this work we develop digitally tunable metasurface with greyscale phase control, enabling active beam manipulation.

**John Castillo**

Program: GRA/Post Masters

School: Georgia Institute of Technology

Group: MST-8

Mentor: Reeju Pokharel

Category: Materials Science

Type: Individual

LA-UR: 19-27030

## **A Fourier Dictionary Approach for Microstructure Reconstruction from HEDM Measurements**

High-energy X-ray diffraction microscopy (HEDM) is a nondestructive technique used for characterizing polycrystalline materials microstructure in three dimensions. The two HEDM techniques, near-field and far-field, are employed to produce measurements which capture the 3-dimensional spatially resolved orientation of a microstructure. Furthermore, due to the non destructive nature of the technique, HEDM measurements provide an opportunity to study microstructures in-situ under various thermo-mechanical loadings. However, the diffraction patterns obtained from HEDM measurements must undergo significant post processing analyses in order to extract the highly valuable spatially resolved orientation information. Currently, the post processing analysis presents the largest bottleneck in the study of HEDM measurements. Current methodologies employ a brute force approach, which require the repetitive forward simulation of diffraction patterns until simulated diffraction patterns match experimentally obtained patterns. In this work, we present a new approach which utilizes the symmeterized generalized spherical harmonics (s-GSH) and the symmeterized surface spherical harmonics (s-SSH) in order to build a compact Fourier based Dictionary. This new approach is expected to greatly reduce the overhead and time necessary to extract the spatially resolved orientation information from HEDM measurements.

**Andre Gouws**

Program: GRA/Post Masters  
School: University of Texas at Austin  
Group: MST-8  
Mentor: Erofilis Kardoulaki

Category: Materials Science  
Type: Individual  
LA-UR: 19-27047

**Selective Laser Flash Sintering of Aluminum Nitride**

Flash sintering allows for the rapid sintering of ceramic components using concurrent applications of furnace heating and electric fields. Selective laser flash sintering (SLFS) uses a laser to selectively heat the surface of a ceramic in order to sinter only specified regions at a time, while simultaneously applying a DC electric field. We have already demonstrated SLFS on 8% yttria-stabilized zirconia. Here we utilize SLFS to demonstrate the ability to initiate sintering of aluminum nitride. We show that at moderate to high combinations of laser flux and field strengths, current flows through the sample. The presence of current is indicative of neck formation. We will present the effects of electric field strength, laser repetitions, laser power, and laser scan speed, and the varying effects on current measured.

## **Rebecca Lalk**

Program: UGS/Postbac

School: Case Western Reserve University

Group: MPA-CINT

Mentor: Paul Dowden

Category: Materials Science

Type: Individual

LA-UR: 19-26677

### **Pulsed Laser Deposition of YBCO Films**

The superconductor, yttrium barium copper oxide (YBCO) crystallizes in a defect perovskite structure and has a transition temperature of 90K, above liquid nitrogen temperature. One of the goals of the Superconductivity Technology Center was to deposit YBCO thick films (~5 microns) via pulsed laser deposition (PLD) with a critical current density above  $J_c = 2.0 \text{ MA/cm}^2$ . However, it was hypothesized that contamination from the braze-alloy assembled heating element and poorly controlled fluence of the excimer laser beam led to reduced current density, off-stoichiometry and repeatability issues in film growths. Now, patented imaged stabilized beam line and braze-free heater allow for more accurate control over deposition parameters and chemical composition of PLD films. The purpose of this project is to return to deposition of YBCO thick films to determine if the aforementioned issues have been solved.

## **Sina Lewis**

Program: GRA/Post Masters  
School: University of Colorado- Boulder  
Group: T-1  
Mentor: Sergei Tretiak

Category: Materials Science  
Type: Individual  
LA-UR: 19-25678

### **Surface Core Level Shifts of Lead Halide Perovskites**

The binding energy of core electrons is highly sensitive to the atom's surrounding chemical environment. Thus, while they don't participate in the chemical reactions, the core electrons can tell us a lot about the chemical composition of the material. Differences in the core electron binding energy of atoms on the surface of a material and those deeper in the bulk are specifically referred to as surface core level shifts (SCLSs). These shifts can provide details about surface adsorbed atoms and other surface details. This is valuable for many materials but of particular interest are the SCLSs of lead halide perovskites which have demonstrated excellent properties for optoelectronic applications yet are extremely reactive in air leading to degradation. Due to the difficulty of experimentally determining these shifts, it remains a challenge to properly assess the condition and composition of synthesized perovskites. We used density functional theory (DFT) calculations as implemented in the Vienna Ab initio Simulation Package (VASP) to quantify the SCLSs of select lead halide perovskites. In addition to examining the chemically clean surface we examine the effect of adding common air molecules (O<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>) as well as molecules commonly used to passivate and protect the perovskite crystal. This research aims to assist in characterizing the surface of these perovskites and guide the development of new methods to protect against degradation.

**Jacob McKenzie**

Program: GRA/Post Masters  
School: University of Oregon  
Group: MST-7  
Mentor: Joseph Torres

Category: Materials Science  
Type: Individual  
LA-UR: 19-26470

## **A Novel Method for Additively Manufacturing Thermosetting Powder Eccostock® on a Benchtop SLS instrument: Sintratec Kit**

A study on additively manufacturing the free-flowing thermosetting powder Eccostock® on a benchtop Select Laser Sintering (SLS) instrument: Sintratec Kit. An extensive cure study was conducted to determine a functional powder bed temperature, utilizing TGA, DSC, and FTIR to quantify degree of cure. The Eccostock® powder was further characterized by REVOLUTION flow analysis, with and without carbon black filler in order to determine flowability and packing density of the powder. By these results, Eccostock® was successfully processed on the Sintratec Kit in the form of compression pads. These pads were analyzed for their compressive strength and degree of cure by DSC, TGA, and SEM. Further work was done in optimizing laser scan speed and hatching distance when processing Eccostock®.

## **Kimberly Pestovich**

Program: UGS/Postbac  
School: New Mexico State University  
Group: MST-8  
Mentor: Kenneth McClellan

Category: Materials Science  
Type: Individual  
LA-UR: 19-26453

### **Development of Polycrystalline Scintillators as a Method to Screen New Compositions Predicted by Machine Learning**

The discovery of new scintillators has historically been accomplished through lengthy trial and error, and the development process for a scintillator optimized for a unique application is labor-intensive. Integrating a physics-based machine learning model to the discovery and development process allows efficient identification of scintillators with properties tailored to a specific application. This type of model identified several compositions within the  $(Y, Lu, Gd)_3(Al, Ga)_5O_{12}:Ce$  garnet family, which were synthesized in the Single Crystal Growth Laboratory. From these compositions, development on  $Y_2LuAl_5O_{12}:Ce$  has continued, including a study examining several different Ce dopant concentrations.

To quickly screen these compositions, polycrystalline ceramic samples were synthesized through two methods: a melt-quench process and co-precipitation. Radiographs taken at the Scintillator Evaluation and Analysis Laboratory allow for relative ranking of the light output of the scintillators, which guides development and informs the machine learning model.

Additionally, the radiographs revealed imperfections in the samples, which gives insight for adjusting synthesis and processing procedures. Irregularities exist in the polycrystalline scintillators, sometimes leading to distinct areas with higher or lower light output compared to the bulk sample. Variations in light output on the different faces of some samples were also seen, possibly related to microstructure since scattering can influence spatial uniformity of measured light. To confidently use high-throughput polycrystalline samples to screen scintillator compositions, consistent properties must be achieved. Changes in sintering temperatures and other processing conditions are being considered to resolve the irregularities.



## **Jaime Regis**

Program: GA/Post Masters  
School: University of Texas at El Paso  
Group: C-CDE  
Mentor: Kwan-Soo Lee

Category: Materials Science  
Type: Individual  
LA-UR: 19-26468

### **Direct Ink Writing of Stretchable Conductive Elastomers**

The use of stretchable electronics has seen a recent increase due to their application in electronic devices and biomedical applications and attracting further attention for their use as stretchable interconnecting electrodes in electronic devices. In this work parametric studies were performed to observe the effects of different Ag flake loading concentrations on the mechanical and conductive, thermal and electrical, properties of 3D printed flexible pads. Different poly(dimethylsyloxane) (PDMS) inks were prepared for 3D printing, varying the weight percent of silver flake particle loadings. Rheological characterization was performed on the inks prior to loading into printer to determine extrudability. PDMS pads designed in face centered tetragonal meshes were fabricated from the different inks using a Hyrel3D System 30M 3D printer. The chemical, thermal, mechanical, and electrical properties of precursors used to prepare the inks and the post-processed materials were characterized. Understanding the correlations between conductivity, elasticity, and concentration of silver flakes will allow quantification of the percolation threshold at which a conductive network is established in the material. Following this would be engineering the interaction between the conductive particles and the matrix material to improve elasticity, allowing for its use in a broader range of applications.

## **Nolan Regis**

Program: GRA/Post Masters  
School: University of Nevada, Las Vegas  
Group: SIGMA-2  
Mentor: Samantha Lawrence

Category: Materials Science  
Type: Individual  
LA-UR: 19-26804

### **Aging Response of Ti-45Nb**

$\beta$ -stabilized titanium alloys, such as Ti-45 wt. pct. Nb (Ti-45Nb), have advantageous properties for biomedical implants, and have potential for use in mission-related applications that require high strength, low density, and predictable corrosion characteristics. Here we investigate the aging response of Ti-45Nb to evaluate alloy performance throughout manufacturing using a suite of analytical techniques. Ti-45Nb specimens were artificially aged at 500 °C between 2 and 144 hours to precipitate and evolve the  $\alpha$ -phase. Prior to aging the material, half of the specimens were cold-rolled to a 5% reduction to study the effects of cold working. A previous aging study on the same material found subtle changes in mechanical response measured with Vickers indentation, tension tests, and compression tests. To supplement and expand on the findings of the previous aging study, the present study uses scanning electron microscope (SEM) and x-ray diffraction (XRD) analysis to characterize changes in microstructure related to artificial aging and cold working. Thus far, preliminary evidence from XRD and SEM analysis reveals a clear relationship between the changes in mechanical response with the evolution of  $\alpha$  in both quantity and morphology. With time, the volume fraction of  $\alpha$  increases, and grains coarsen in both cold-rolled and non-cold-rolled specimens. However, distinct morphological differences between the cold-rolled (smaller, uniformly distributed grains) and non-cold-rolled (larger, coarse needle-like grains) samples is evident in SEM. To quantify these SEM observations, XRD analysis on the remaining aged samples is planned.

## **Cameron Richards**

Program: GRA/Post Masters

School: University of Oregon

Group: MST-7

Mentor: Brenden Wiggins

Category: Materials Science

Type: Individual

LA-UR: 19-26353

## **Optical Properties of BaFCl:Eu<sup>2+</sup>-Scintillating Composites for Medical X-ray Imaging Applications**

X-ray computed tomography (CT) scanners are critical diagnostic tools in the medical industry that have been shown to be extremely effective for studying the internal structures of patients. Though invaluable, the CT technique tends to be expensive due to equipment costs and operational time investments. Therefore, a cost effective approach for improving image quality while reducing operational time requirements is presented. A translucent scintillating composite, composed of Eu(II)-doped BaFCl and optical adhesive of similar refractive index, is shown to be an attractive alternative to current state-of-the-art materials for X-ray detection, at a fraction of the developmental costs. Additionally, a pixelated detector approach, utilizing the BaFCl:Eu<sup>2+</sup> composite, can significantly improve the overall spatial resolution and image quality. Through this research, BaFCl:Eu<sup>2+</sup> synthesis parameters and composite compositions were optimized to balance scintillation properties, translucency, and viscosity. The optimal composite composition displayed bright luminescence under UV and X-ray irradiation, maintained visible light propagation, and can be easily applied into small pixelated structures. Based on these results, this technology can reduce the cost of operation, provide excellent image quality, and reduce the required X-ray dose given to the patient.

## **Natalia Rubio**

Program: UGS/Postbac

School: University of California, Berkeley

Group: MST-8

Mentor: Stuart Maloy

Category: Materials Science

Type: Individual

LA-UR: 19-26496

### **Corrosion of Refractory Metals in High Temperature LBE**

LBE (Lead-Bismuth Eutectic: 44.5 wt% Pb, 55.5 wt%Bi) is an attractive coolant and spallation target for nuclear systems because of its advantageous qualities: a wide liquid phase, high thermal conductivity, high density, inertness in air and water, small solidification volume change, and very low neutron moderation. A significant drawback of LBE is its corrosivity, which necessitates a compatible structural material. In this work, several refractory metals (Nb, Ta, Mo, and TZM) are investigated for their corrosion resistance in high-temperature LBE. Samples of each metal were exposed to stagnant LBE at 700°C and saturation oxygen concentration for one week at Niowave Inc, Lansing, MI. They were then analyzed for corrosion damage at LANL through cross-sectional analysis using SEM and optical microscopy. Similar studies had been done previously, but it was difficult to determine the extent of the corrosion damage without a “zero corrosion” baseline mark to compare to. In this analysis, a section of each sample was coated with titanium nitride before exposure to LBE to shield it from corrosion and provide a benchmark against which to compare the corroded sections.

## **Chih-Feng Wang**

Program: GRA/Post Masters  
School: University of New Mexico  
Group: MPA-CINT  
Mentor: Houtong Chen

Category: Materials Science  
Type: Individual  
LA-UR: 19-26911

### **Nano-FTIR Spectroscopy of Intersubband Transition in Single Plasmonic Nanoantenna Regime**

The intersubband transition (ISBT) between ground state to excited state in the semiconductor heterostructures enable a variety of devices, i.e. quantum cascade laser, and photodetectors from far-to near- infrared. Interesting quantum phenomena reveal when ISBT strong coupled with a subwavelength plasmonic nanoantennae such that ISB electronic excitation forms a coherent superposition with the photon field, known as ISB polaritons. This light-matter interaction leads to unexplored regime of ultra-strong coupling. However, experimental observation of ISB polaritons in an isolated nanoantenna has not yet been reported due to the challenging of spatial resolution in the subwavelength. Here, we combined the techniques of scattering scanning near-field optical microscopy (s-SNOM) and Fourier-transform infrared (FTIR) spectroscopy, named nano-FTIR, to detect the formation of ISB polariton states in a single nanoantenna. The nanoantenna was excited by a broadband IR pulse and spectrally analyzed evanescent fields on the nanoantenna surface with 25 nm spatial resolution. We are the first successful observation on the ISBT coupled to a single nanoantenna, that strong coupling reveal the distinctive splitting of the nanoantenna resonance peak into two polariton modes with two  $\pi$ -phase steps corresponding to each of the modes. Furthermore, ISB polariton dispersion was mapped using a set of nanoantennae that the resonance frequencies was tuned with different sizes. This nano-FTIR spectroscopy approach opens doors for investigations of ISB polariton physics in the single subwavelength nanoantenna regime and will assist developing of practical applications such as IR metasurfaces.

## **Jon Doorn**

Program: UGS/Postbac  
School: Purdue University  
Group: MPA-MAG  
Mentor: Scott Crooker

## **Ingrid Zimmermann**

Program: UGS/Postbac  
School: Rutgers University  
Group: MPA-MAGLAB  
Mentor: Ross McDonald

Category: Materials Science  
Type: Group  
LA-UR: 19-27041

# **High Magnetic Field Photoluminescence and Magnetotransport Measurements on a 2D Electron Gas**

GaN is a semiconductor material which is becoming increasingly utilized in technological applications and is known for its large bandgap, effective mass, and high electron mobilities. We measure the behavior of a two-dimensional electron gas (2DEG) confined in a GaN/AlGaN semiconductor heterostructure by performing both photoluminescence spectroscopy (PL) and magnetotransport measurements at high magnetic fields. PL and transport measurements in pulsed fields up to 60 T have been made separately. However, we noticed that the presence of light changes the carrier density of the GaN sample, which we observed through changes in the resistance and change in the frequency of quantum oscillations before and after it was exposed to light. This called for the measurement of the sample using PL and transport techniques simultaneously, which we conducted in a superconducting magnet up to 15 T, enabling us to precisely control the sample's exposure to light. Quantum oscillations of the same frequency can be seen in results from both techniques, which is due to the spreading of Landau levels in the magnetic field. We experimented with different intensities and wavelengths of light to see how this affects the carrier density of the heterostructure and to determine whether we could tune the carrier density below its typical value when not illuminated.

# **MATHEMATICS**

## **Ian Gallagher**

Program: GRA/Post Masters

School: University of Bristol

Group: A-4

Mentor: Melissa Turcotte

Category: Mathematics

Type: Individual

LA-UR: 19-27048

### **Anomaly Detection in Computer Networks via Spectral Embedding**

One approach to cyber-security is to create signatures for known attacks so they are detected whenever they appear on our network. However, we also want to spot and quarantine new malicious behavior as it happens, rather than solely waiting for a update to our anti-virus software.

In this poster, we analyze LANL netflow records of users accessing computers over a three month period. Due to the nature of computer activity, including, but not limited to, work/home pattern of life, burstiness of activity online and periodic automated activity, pretty much any computer activity appears anomalous. The high levels of false positives when modeling the behavior on any connection makes such an approach impractical for large networks.

One solution to this problem is to accumulate weak evidence into something much stronger. We do this by constructing a graph between user and computer nodes. An edge in this network could represent the number of connections between a user and a computer, whether any connection happened at all, or the probability those connections are anomalous according to some model [1]. We analyze this graph by embedding the nodes into a lower dimensional space by the eigenvalue decomposition of the graph adjacency matrix. Under certain model conditions, for example, fixed roles for users and computers in the network, we have a Central Limit Theorem for the position of nodes in the latent space [2]. By analyzing these positions, and how they move over time, we can locate anomalous users and computers in the network with fewer false positives.

[1] Turcotte, Melissa, et al. "Poisson factorization for peer-based anomaly detection." 2016 IEEE Conference on Intelligence and Security Informatics (ISI). IEEE, 2016.

[2] Rubin-Delanchy, Patrick, et al. "A statistical interpretation of spectral embedding: the generalised random dot product graph." arXiv preprint arXiv:1709.05506 (2017).



### **Philippa Chadwick**

Program: UGS/Postbac  
School: Bard College, NY  
Group: A-1  
Mentor: Sara Del Valle

### **Oscar Goodloe**

Program: UGS/Postbac  
School: Arizona State University  
Group: A-1  
Mentor: Geoffrey Fairchild

### **Nilesh Mukundan**

Program: High School  
School: Los Alamos High School  
Group: A-1  
Mentor: Sara Del Valle

Category: Mathematics  
Type: Group  
LA-UR: 19-26999

## **Quantitative Predictors of Political Instability in Pakistan**

This project assesses the relevant and impactful indicators for political instability in Pakistan. These indicators were selected through a systematic literature review looking at the causes of political instability on a global scale. To specify the literature review to Pakistan, country-specific searches were conducted to define which indicators were the most important for Pakistan and the region. Once indicators were compiled, the principal goal of the project in this early stage was the identification, collection, curation, and preliminary analysis of data streams for these indicators to determine which are practical in a modeling context. While a comprehensive selection of data streams representing each indicator has not yet been assembled, data was found for some key predictors, namely occurrences of terror events, violence history, changes in leadership, and forest coverage. Using these predictors, we developed a preliminary model of political instability utilizing a random forest model. The model shows promise as a preliminary step, and could conceivably improve with more predictors. The overall goal of this project is to eventually develop regional political instability models that will provide near real-time political instability forecasts with quantified uncertainty. Despite the extremely complex state space for instability processes and their predictors, early results indicate that data-centric approaches to instability modeling have great potential in predicting and understanding political instability.

**OTHER (NON-TECHNICAL)**

## **Ian Canfield**

Program: UGS/Postbac  
School: University of Texas at Austin  
Group: NEN-1  
Mentor: Johnna Marlow

Category: Other (Non-technical)  
Type: Individual  
LA-UR: 19-26634

### **NMAC for Practitioners 2018**

In August 2018, the IAEA launched NMAC for Practitioners, a practical course in Nuclear Material Accounting and Control (NMAC) to help international nuclear material custodians prevent unauthorized activity by non-state actors. While taught and designed by IAEA officials, the bulk of the course material was developed by the Nuclear Engineering and Nonproliferation Safeguards Science and Technology Group here at LANL. Over the course of the summer, I helped the team develop and test various aspects of the course. In August, I helped set-up the schoolhouse and participated in the first week of lectures before returning to school.

In June, I made the final edits to the lecture slides for the course. This involved incorporating comments from various international experts involved with the project. It was a fascinating look into the way collaboration is done behind the scenes on complex multinational projects.

My most important role was to craft a capstone exercise to finish the course. The exercise involved four teams of six participants performing a mock Physical Inventory-Taking (PIT) of a vault (including actual Special Nuclear Material to characterize), during which they would discover an irregularity and work out how to resolve it. The basic premise of each activity had been laid out by DOE and IAEA designers before I arrived, so I prepared props and wrote the procedures and forms that guided participants and their supervisors through the exercise. I spent a fair amount time in the lab with my mentor testing and refining these materials.

At 24 foreign national participants, the course was the largest ever taught at the TA-66 Schoolhouse. It was a resounding success and the IAEA has decided to run it again with 42 participants in April 2020. I am currently expanding the capstone exercise for use by the larger group.

## **Anjeli Doty**

Program: UGS/Postbac  
School: Montana State University  
Group: CAP-CAS  
Mentor: Kirsten Fox

Category: Other (Non-technical)  
Type: Individual  
LA-UR: 19-26727

### **Optimizing Multimodal Science Communication in a Government Organization**

Science communication at Los Alamos National Laboratory (LANL) is diverse and multifaceted, with numerous and sometimes disparate goals, audiences, and platforms. Unique challenges and opportunities arise as science communicators tailor strategies and products to divergent objectives and platforms, vis-à-vis a broad range of outreach needs and ongoing. Finding solutions for each distinctive problem requires innovation and responsive flexibility. In LANL's Earth and Environmental Sciences division, science communications span a range from developing modernized website content; to creating multimodal promotional material for international research campaigns; to designing presentations for upper-level Department Of Energy programmatic reviews; to creating news articles customized for internal and external audiences; to authoring technical science highlights. As a science communications intern for the past year working with my mentor Kirsten Fox, I have observed patterns of governmental laboratory communication, and developed responsive strategic methods of approaching and solving challenges. Although communication goals vary cross-organization as each customer brings specific requirements, certain features of impactful science communications remain consistent. These include an ability to identify and navigate contextual communicative features and constraints; perpetually oscillate between big-picture strategy and detail-oriented tasks; and cultivate the professional empathy needed to understand and engage different types of individuals in order to convey accurate information through optimal channels. Much of the science communicator's role is identifying and building out the space between divergent audiences while remaining "on message." Even as LANL scientists are committed to the technical accuracy of their research, the lay public desires and deserves comprehensive communication from the Lab, particularly as a taxpayer-funded institution. The dissemination of knowledge propels global progress. Successful science communication at LANL occur as communicators find shared ground between the needs of diverse audiences to determine the most efficacious platform to create and deliver unified messages in support of a distinguished public image of LANL.

## **Sarah Hayes**

Program: GRA/Post Masters

School: University of Illinois at Urbana-Champaign

Group: SRO-RL

Mentor: Michelle Mittrach

Category: Other (Non-technical)

Type: Individual

LA-UR: 19-25952

## **Performing Library Outreach for Excellence in Community Relations at Los Alamos National Laboratory**

The Los Alamos National Laboratory's Research Library is dedicated to providing essential knowledge services that enable delivery of innovative science and technology to protect our nation and promote world stability. However, despite being an access point for scientific literature and research instruction and also being the only Department of Energy lab library open to the public, the Research Library is actively working to improve its presence within LANL and the greater Los Alamos community. Through qualitative research involving one-on-one communication with community members, we have reached two points regarding library outreach: Los Alamos community members are aware of the Research Library but assume it is closed off to non-lab employees; Los Alamos employees are not aware the Library exists within the JRO Study Center, or associate it with non-library functions in the same building (e.g. Cryptocard activation, conference room reservations). To combat these perceptions and increase visibility for the Research Library, we have put into action several outreach efforts: a postcard project promoting the library for multiple patron sets; paper brochures promoting the library's services; a working relationship with the Los Alamos County Library with plans for cross- promotion and joint programming; passively interactive in-library display tables based on timely themes (e.g. Fair Use Week, Earth Week).

## **Rebecca Wantuck**

Program: UGS/Postbac

School: Fort Lewis College

Group: OSH-OH

Mentor: Martha Kwan Yi Chan

Category: Other (Non-technical)

Type: Individual

LA-UR: 19-26658

### **Glovebox Worker Dexterity in Overgloves**

At Los Alamos National Laboratory (LANL), approximately 500 gloveboxes are used for different applications, of those, approximately 400 gloveboxes reside in the Plutonium Facility in TA-55 (PF-4), utilized mainly for nuclear material processing. Gloveboxes present a number of ergonomic hazards including awkward posture and repetitive motions. This study focused on the repetitive motions of the hand, specifically looking at worker dexterity performance and glovebox glove/overglove combination. While the glovebox glove is the weakest component of safety in a containment perspective and ergonomics in a human operation perspective, it is also the easiest part of the glovebox to change. The aim of this study was to address a lack in overglove dexterity research and to help in future design glovebox processes to improve safety, worker comfort and productivity.

33 experienced glovebox workers performed three dexterity tests and two measures of hand strength in this study. Participants completed the tests with 30mil lead-lined glovebox gloves alone and 30mil lead lined gloves with overgloves. Results of this study shows that the overgloves usage increased task time by approximately 20-30%. The overgloves diminished the grip strength of the individual by approximately 20% and the pinch strength by approximately 10%.

### **Asif Ali**

Program: UGS/Postbac  
School: University of Illinois at Urbana-Champaign  
Group: SRO-RL  
Mentor: Tebols Casados

### **Thomas Chadwick**

Program: UGS/Postbac  
School: University of California, Berkeley  
Group: WRS-SIS  
Mentor: Alan Carr

### **Andrew Port**

Program: UGS/Postbac  
School: Norwich University  
Group: WRS-SIS  
Mentor: Danny Alcazar

Category: Other (Non-technical)  
Type: Group  
LA-UR: 19-25700

## **Building a Digital Historical Narrative Using Open-Source Tools**

When building educational material for the public, institutions have several tools at their disposal. Open source tools particularly appeal to libraries thanks to their low cost and ability to integrate with library systems. One platform, Omeka S, is of particular interest to the Los Alamos National Laboratory Research Library. This project intends to showcase how open source tools such as Omeka S can be used to build digital historical narratives by cataloging and publishing digitized collections. As a proof of concept, an Omeka S website was built which showcases a digitized collection and historical narrative about photography and cinematography of atmospheric nuclear weapons tests.

## **Lauryn Anaya**

Program: UGS/Postbac  
School: University of New Mexico  
Group: ALDCP  
Mentor: Lynn Clarkson

## **Elif Oguz Erkal**

Program: GRA/Post Masters  
School: University of Colorado Boulder  
Group: INNO-ASSUR  
Mentor: Steven Renfro

Category: Other (Non-Technical)  
Type: Group  
LA-UR: 19-25767

## **Learning Organizations in Capital Projects**

At its simplest form, organizational learning is defined to be the creation, storage and mobilization of knowledge within organizations that has a considerable impact on an organization's performance. Organizational learning, knowledge and innovation management have been studied heavily through the lens of private business optimization for various industries, however, such an approach has not yet been studied in a National Laboratory, especially in construction. Publicly funded design and construction organizations, such as Capital Projects at Los Alamos National Laboratory (LANL) could benefit from a better understanding of organizational learning, knowledge and innovation management systems. It has been challenging to establish such systems in the construction industry due to its unique, complex, multi-stakeholder, multi-trade, high turnover nature and the variety of authentic complications simultaneously occurring at project sites. This research strives to understand organizational learning status within construction project settings through interviews, focus groups, surveys and a literature review. Literature on Learning Organization Rapid Diagnostic Tool (LEONARDO) was used as an initial benchmarking study performed for historical comparison of Capital Projects to various other organizations on the aspect of organizational learning. This research includes an elaborate case study of Capital Projects presenting the methodology used to understand the organizational learning attributes of an organization while demonstrating its applicability and replicability in LANL as a whole. This initial attempt to understand knowledge and innovation management systems could be used by Capital Projects to restructure for increased efficiency and performance as a first step to improve and suggest better practices for an organizational learning action plan development process. The subsequent steps are to apply an organizational assessment framework to LANL as an institution and come up with applicable action plans to follow. Additionally, the findings of this research will be applied in additional studies for a PhD dissertation henceforth.



## **Shay Archuleta**

Program: UGS/Postbac  
School: New Mexico State University  
Group: SI-DC  
Mentor: Yvonne Archuleta

## **Kaylee Maes**

Program: UGS/Postbac  
School: University of New Mexico- Los Alamos  
Group: SI-DC  
Mentor: Yvonne Archuleta

Category: Other (Non-technical)  
Type: Group  
LA-UR: 19-26364

## **TA-18 Records Preservation Project**

The TA-18 Records Preservation Project is of great importance to all of Los Alamos National Laboratory (LANL). TA-18 (also known as Pajarito Site) was one of the first Technical Areas (TAs) built in the 1940's when LANL was established. During the Manhattan Project time period at LANL, TA-18 was used as an artillery and explosives ordinance test range. In 1946 after Louis Slotin received a lethal radiation exposure from an experiment gone wrong, this TA was chosen as the main location for performing remote nuclear critical assembly operations which became known as the Los Alamos Critical Experiments Facility (LACEF). After WWII and throughout the Cold War, the buildings at TA-18 housed the performance of many projects that hold significant importance and history to our nation's nuclear security. The research included nuclear weapons safety studies, nuclear materials criticality safety research, nuclear rocket propulsion research, diagnostic instrument development for the Nuclear Emergency Search Team (NEST), and the development of other health and safety protocols associated with the safe handling of special nuclear materials. Because it was an aging facility and ultimately for security reasons, it was decided that experimental capabilities at TA-18 be moved to a new location. Once the capabilities were relocated, a decision was made to demolish most of the buildings. Some of the buildings were spared the demolition fate because of the site's historical significance. As is the case for many older TAs at LANL, there exist many important records and documents that require preservation. In accordance with DOE's records policies, it was of most importance that these records get properly archived. Not only do these records provide historical importance, but when they are properly archived, scientist today and for future generations will have access to these experiments etc. that are from the very beginning of LANL.

### **Isaiah Gurule**

Program: UGS/Postbac  
School: New Mexico Tech  
Group: EPC-WMS  
Mentor: Steven Singledecker

### **Jonathan Sanchez**

Program: UGS/Postbac  
School: Adams State University  
Group: EPC-WMS  
Mentor: Maryrose Montalvo

### **Richard Sandoval**

Program: UGS/Postbac  
School: Eastern New Mexico University  
Group: EPC-WMS  
Mentor: Steven Singledecker

Category: Other (Non-technical)  
Type: Group  
LA-UR: 19-25698

## **The Future of Waste Tracking Operations at Los Alamos National Laboratory**

Waste Management Services (EPC-WMS) coordinates the disposition of non-hazardous, hazardous, chemical, and radioactive wastes, and provides services to waste generators with a commitment to LANL environmental policies. To do so, EPC-WMS employs a variety of robust tools and initiatives to track waste packaging and shipping activities, and divert waste wherever possible. Managing and reducing the Laboratory's waste stream is tracked as a performance measure. The Laboratory's waste characterization and tracking software, (WCATS), hand-held batch data collection units such as the LDX10, and recycling as a waste minimization strategy, are the key focuses of this poster.

## **Hunter Swavely**

Program: High School  
School: Los Alamos High School  
Group: EPC-WMP  
Mentor: LeAnn Purtzer

## **Elijah Velasquez**

Program: UGS/Postbac  
School: Queens University of Charlotte  
Group: EPC-Wmp  
Mentor: LeAnn Purtzer

Category: Other (Non-technical)

Type: Group

LA-UR: 19-26806

## **The future of waste management and reduction shows promise with technological advances that have sparked newer and more efficient methods**

The safe, clean, and efficient reduction and management of both radioactive and nonradioactive wastes are essential processes, however, these processes can be time consuming, complicated, and costly. The goal of this poster is to research possible waste solutions that will encourage the use of more environmentally and monetarily efficient methods of waste disposal, and decrease the amount of hazardous waste bound for energy recovery, treatment, and disposal facilities. Technological advances such as smart trash bins provide a more efficient means of disposing solid wastes and encouraging recycling. Using artificial intelligence, these bins are able to categorize and separate different forms of waste and recyclable material. The smart bins also provide a method for ensuring the most efficient pick up times for waste facilities. This is done with the use of trash bin sensors, thus, overtime saving money and reducing CO2 emissions. Some countries are also finding ways on a larger scale to reduce waste and encourage environmentally friendly practices. Facilities are reducing waste output through waste recycling, and they are using the waste-to-energy techniques to supply cities with the majority of needed energy. The adoption and encouragement of technological advances in waste reduction and energy restoration can lead to a diminished need for hazardous waste treatment plants, and have a significant impact on preserving our resources, protecting the environment, and simultaneously reducing costs over time.

# **PHYSICS**

## **Ethan Aulwes**

Program: UGS/Postbac

School: Dartmouth

Group: P-23

Mentor: Michelle Espy

Category: Physics

Type: Individual

LA-UR: 19-26073

## **Developing a Treatment Planning Method for High-Energy Proton Therapy**

Ethan Aulwes, Matthew Freeman, Frank Merrill, Dale Tupa, Michelle Espy

Proton therapy is an established cancer treatment technique that has demonstrated improved patient outcomes, due to improvements in dose deposition accuracy. Similar to other types of radiotherapy, it involves bombarding the target tumor with particles that deposit energy, namely protons in this case, which kill cancerous cells. However, those protons also damage any healthy cells that they deposit energy in, and thus there is a need to be as accurate as possible with dose delivery. A proton beam deposits the bulk of its dose at the end of range in what is known as the Bragg peak. This Bragg peak makes possible the treatment of tumors located near sensitive or vulnerable tissue, but the fine-tuning of proton therapy requires careful treatment planning and knowledge of a patient's specific anatomy. MatRad is a free open-source software that provides methods of dose optimization for various treatment plans using contoured CT data of tumor sites and surrounding organs at risk (OAR). This software will be used to compare the optimized treatment plans of proton and photon therapy by examining their expected dose to target tumor and OAR regions. Using CT data sets of tumors located in a patient's head and another patient's prostate, the goal is to evaluate which treatment plan anticipates less dose to the healthy tissue and the most constrained dose to the target. The effectiveness of dose optimization can be examined with dose-volume histograms showing the percent of tissue volume exposed to certain levels of radiation. Finally, a treatment plan will be designed for high-energy relativistic protons produced by the accelerator at LANSCE and compared to treatment plans for proton energies common at medical treatment facilities.

**Naia Butler-Craig**

Program: GRA/Post Masters  
School: Georgia Institute of Technology  
Group: CCS-2  
Mentor: Nicole Lloyd-Ronning

Category: Physics  
Type: Individual  
LA-UR: 19-26489

## **Particle-in-cell simulation of plasma confinement in Hall-Effect Thruster channel**

The work outlined in this paper used particle-in-cell kinetic codes to simulate the stability of plasma in the channel of Hall-effect thrusters with ranging surface-area-to-volume (SAV) ratios and power levels (including sub-kilowatt). Based on the results of the iterations, the plasma characteristics that minimized plasma-wall interactions were identified. The purpose of this research is to determine the conditions under which electron flow is adequately confined in the channel of the thruster, subsequently extending the life-time of the thruster. The variables explored are: power levels ranging from 500 W to 2 kW, SAV ratios ranging from 2 to 4, and plasma characteristics ranging from mass ratio, volume flow rate (speed), and ionizing energy. Ideal conditions for plasma characteristics like ion-to-electron mass ratio were noted to recommend propellant most suitable for confined electron flow. Findings include that krypton gas provided the ideal mass ratio.

## **Anna Cooleybeck**

Program: UGS/Postbac  
School: University of Michigan  
Group: AOT-AE  
Mentor: Bruce Carlsten

Category: Physics  
Type: Individual  
LA-UR: 19-26626

### **Modeling a high-efficiency klystron**

Klystrons are microwave sources most commonly used to supply the input signal for large particle accelerators, as well as for a variety of other uses including communications, radar, and medicine. As accelerator technology advances, microwave sources with better efficiencies are required, up to or exceeding 80%. Klystron operation relies on a bunched electron beam, where electrons group together in coherent packets rather than spreading out into a continuous beam. For high efficiency, we require a high degree of bunching and a low longitudinal energy spread within these bunches. A proposed way to achieve this is to hold a portion of the klystron at a lower voltage. As the electron beam passes this voltage-depressed section, it decelerates, then re-accelerates to its original energy, leading to the high bunching and low energy spread desired. To evaluate this approach, a design for a klystron with voltage depression is developed using the particle-in-cell code TUBE. This design is then analyzed further to determine whether the high bunching and low energy spread can be maintained past the voltage depression and to evaluate effects on the overall efficiency.

**Katherine Elliott**

Program: UGS/Postbac

School: James Madison University

Group: T-1

Mentor: Mark Zammit

Category: Physics

Type: Individual

LA-UR: 19-26877

## **Collisional Line Broadening in Hydrogen and Helium White Dwarf Atmospheres**

White dwarf stars in the Milky Way are characterized by their atmospheric temperature, composition and surface gravity. This information can be utilized to determine the history of star formation in our Galaxy. One way to determine the effective temperature of a white dwarf star is by utilizing the line-ratios of atomic hydrogen. The gravity can be deduced from the line width caused by various broadening processes. Recently, a white dwarf star was observed with skewed, hydrogen transition lines, which is indicative of collision broadening by a new process. It is hypothesized that this anomaly is a result of a dense atmospheric mixture of hydrogen and helium atoms. During this project we are working towards determining the theoretical line position and line shape profile for the hydrogen+helium collision system. Utilizing the Quantum Chemistry package MOLPRO, we studied the excited states of HeH using a variety of active spaces, basis sets and Rydberg functions to obtain the corresponding converged potential energy curves and dipole moment curves. In the future, these quantum chemistry calculations will be used to determine the theoretical line position and shape for hydrogen+helium collisions. These results will be included in a white dwarf spectrum calculation to compare with the observed spectrum of the white dwarf with the anomalous asymmetric hydrogen line profiles.



## **Onnolee Erickson**

Program: UGS/Postbac  
School: Stony Brook University  
Group: P-23  
Mentor: Amanda Gehring

Category: Physics  
Type: Individual  
LA-UR: 19-26894

### **Calibrating Image Plates with Bismuth-207**

The purpose of this project was to create an efficient method for calibrating image plates (IPs) after they were irradiated by Bismuth-207 for varying amounts of time. A method was created in order to determine the amount of energy that the Bismuth-207 deposits and how the time of exposure affects the energy dissipated. Bismuth-207 has a half-life of 31.55 years and decays by electron capture, where an electron is captured by the nucleus and a neutrino is emitted. IPs are advantageous for digitizing the energy deposition from a radioactive source. The energy is stored in the IP and released once the IP is scanned in an IP scanner, which relies on the principle of photostimulated luminescence. The released energy is then amplified by a photomultiplier tube that is internal to the IP scanner, which then digitizes the signal. We analyze the digitized data in order to determine the energy deposited by the source and how it corresponds to the signal measured by the IP reader. The analysis code detects the areas on the IP where the source was placed, with minimal user input, and subtracts the background from the original image to create an image without background. The image without background is then used to determine the correlation between the energy deposition of the Bismuth-207 and the known time the IP was exposed to the source. I will present the details of the calibration and experiment as well as multiple examples that highlight the usefulness of the calibration

## **William Gammel**

Program: GRA/Post Masters

School: University of Arizona

Group: XCP-6

Mentor: Joshua Sauppe

Category: Physics

Type: Individual

LA-UR: 19-26117

## **Sensitivity of the Convergence to Direct-Drive Cylindrical Implosion Parameters**

To achieve efficient thermonuclear burn in Inertial Confinement Fusion (ICF) implosions, high convergence is needed to reduce the required amount of driver energy. Additionally, there is a well-known correlation between the convergence and hydrodynamic instabilities, such as the Rayleigh-Taylor (RT) instability, which have a deleterious effect on ICF. Thus, examining both the consequences of high convergence as well as the target parameters necessary for achieving this condition is essential to the development of robust target designs.

1D simulations of cylindrical targets produced by the Los Alamos Eulerian radiation- hydrodynamics code, xRAGE, have been used to search our target parameter space. Studying the topology of these spaces both informs our understanding of the sensitivity of the convergence to target design parameters, such as fill density, and provides insight into the exact extent to which instability growth can be attributed to convergence.

We will present future plans for high convergence direct-drive cylindrical implosion experiments fielded at the National Ignition Facility (NIF). Experiments utilizing the NIF should be able to produce high quality measurements reaching convergences near 15; 4x greater than previous cylindrical implosions.

## **Austin Gilbert**

Program: GRA/Post Masters  
School: Michigan State University  
Group: CCS-2  
Mentor: Jeffrey Haack

Category: Physics  
Type: Individual  
LA-UR: 19-27090

## **Significant Parameters for Classifying Hydrodynamic Breakdown in HED Plasmas**

Correct prediction of shock width is important for evaluating atomic mixing in high energy density plasma experiments, e.g. shell-fuel mixing in inertial confinement fusion capsules. In this study we use machine learning to attempt to identify when 1d fluid descriptions of a multi species plasma reminiscent of a capsule interface fail to adequately describe a standing shock, and determine when a kinetic description is appropriate. We compare the effectiveness of various combinations of several different metrics for non-equilibrium behavior, such as shock width, species mixing, temperature anisotropy, knudsen numbers, and deviations from maxwellian distributions between a fluid and kinetic model to efficiently train a perceptron identify the breakdown regime.

## **Elena Gonzales**

Program: UGS/Postbac  
School: New Mexico State University  
Group: ISR-2  
Mentor: Ernst Esch, Caleb Roecker

Category: Physics  
Type: Individual  
LA-UR: 19-26472

### **PMT Pulse Characterization**

For nearly 70 years, photomultiplier tubes (PMTs) have been used to measure the response of scintillation detectors to ionizing radiation. In a PMT, photons strike the photocathode and are converted to electrons, which travel through a dynode string, that acts as an electron multiplier, and end in the anode. Due to consistent performance and radiation hardness, PMTs find wide use in nuclear physics experiments.

While most photomultiplier tubes detect a single photon interaction in the scintillator, our experiment operates in a flash detection mode measuring multiple photons in a short period of time. This level of light incident upon the PMT has the potential to produce a non-linear response. To characterize our PMT response at varying light levels as a function of voltage, we have designed an experimental setup consisting of two photomultiplier tubes attached to the same scintillator. One PMT was used as a control, operating at a low and fixed voltage. Its output was connected to a CSA to amplify and integrate the waveform before reaching a digitizer. The independent PMT was operated at different voltages and the output was directly digitized.

To characterize the independent PMT response, a LASER was shot into the scintillator at varying light levels and the response was recorded on the control PMT. For each laser light level, the independent PMT voltage was swept over its operating voltage range. The ratio of the independent to control PMT response was characterized as a function of the LASER light level and the independent PMT voltage to produce response curves.

## **Samuel Matthew Greess**

Program: GRA/Post Masters  
School: University of Wisconsin  
Group: T-5  
Mentor: Adam Stanier

Category: Physics  
Type: Individual  
LA-UR: 19-25688

### **Understanding magnetic reconnection in space using laboratory experiments and simulation**

Magnetic reconnection is a plasma process that occurs at the magnetopause, the boundary between the Earth's magnetic field and the solar wind. Field lines from these two systems merge together, break, and reform into new field lines that allow solar wind particles to travel into the Earth's atmosphere. This process is responsible for the aurora and other space weather phenomena, and in some circumstances it can damage satellites or even cause large-scale power outages. Magnetic reconnection is studied in situ by satellites such as those in the Magnetospheric Multiscale Mission (MMS), as well as in more controlled and reproducible situations like experiments and simulations. The Terrestrial Reconnection EXperiment (TREX), a DoE User Facility at the University of Wisconsin, is optimally designed to reach the parameter regime that characterizes magnetopause reconnection. The new cylindrical geometry capability for the LANL Vector Particle-In-Cell (VPIC) code allows the TREX geometry to be modeled from first-principles with all of the relevant physics. Results from VPIC have shown excellent agreement with the measurements from TREX, and both of these methods have revealed reconnection current layers on the order of  $2-3 d_e$ , where  $d_e$  is the electron inertial length; this is in contrast to prior experiments, which have disagreed with simulation data by asserting that the layer width in magnetopause-like reconnection is several times thicker.

S. Greess, J. Egedal, University of Wisconsin, Madison, A. Stanier, W. Daughton, Los Alamos National Laboratory

## **Abigail Hsu**

Program: GRA/Post Masters  
School: Stony Brook University  
Group: XCP-6  
Mentor: Baolian Cheng

Category: Physics  
Type: Individual  
LA-UR: 19-25674

### **Analysis of NIF scaling using physics informed machine learning**

Hundreds of thermonuclear (TN) ignition experiments in inertial confinement fusion (ICF) were conducted on the National Ignition Facility (NIF) in the last eight years. None of the experiments achieved ignition. In fact, the measured neutron outputs from the experiments were far below what was expected. Although experiments to fine-tune the target designs are the focus of the national ICF program, insightful analysis of the vast amount of existing data is a pressing need. In highly integrated ignition experiments it is impossible to vary only one design parameter without perturbing all other implosion variables. Thus, to determine the nonlinear relationships between the design parameters and performance from the data, a multivariate analysis based on physics model is necessary. We apply the machine learning methods to the existing NIF experimental data to uncover the patterns and physics scaling laws in TN ignition. In this study, we focus on the scaling laws between the implosion parameters and neutron yield by using different supervised machine learning methods include Polynomial Regression, Connected Neural Network, and Deep Jointly-Informed Neural Network developed by LLNL. Our results show that these models are able to predict the outcomes reasonably well from the trained experimental data. Predictions are in good agreement with data and theory. This exploratory study will help build new capability to evaluate capsule designs and provide suggestions for new designs.

**Sara Hurd**

Program: UGS/Postbac  
School: New Mexico State University  
Group: P-21  
Mentor: Malcolm Boshier

Category: Physics  
Type: Individual  
LA-UR: 19-26993

## **Optimizing Transport of Cold Atoms**

When atoms become extremely cold, they form a state of matter known as a “Bose- Einstein condensate” (BEC). Atoms in this state are useful for making sensors because microscopic quantum phenomena, particularly wave function interference, become apparent. This can be exploited to build ultrasensitive navigation systems.

After their temperature is reduced by laser cooling, the atoms must be transported to an interaction region. The transport is accomplished by trapping BEC’s in a focused laser beam using their electrical polarizability and moving the focal point. It is extremely important that the atoms are not significantly heated during the transport. My project is to model the transport of atoms in the optical tweezer, to find trajectories which would minimize excitations of the atoms. I have simulated and analyzed this process using classical mechanics.

Near the bottom of the trap, the potential can be approximated as a simple harmonic oscillator, which allows the problem to be solved analytically. My poster compares the harmonic oscillator approximation to the numerical simulation for the real potential to determine if there are significant differences in their predictions for heating of the atoms. My results are being tested and used in a cold atom experiment in P-21.

## **Travis Jones**

Program: GRA/Post Masters  
School: Georgia Institute of Technology  
Group: C-PCS  
Mentor: Pamela Bowlan

Category: Physics  
Type: Individual  
LA-UR: 19-26946

## **Measuring Femtosecond Extreme-Ultraviolet Pulses With Slow Visible Cameras**

The measurement of light has led to many important scientific discoveries. In particular, the advent of bright, coherent sources of ultraviolet (UV) to extreme UV light pulses, could enable us to study the dynamics of a wide variety materials with nanometer spatial resolution, and as short as attosecond temporal resolution. However, in order to use these sources effectively, it is essential to be able to measure the complete electric field,  $E(t)$ , of their pulses.

Frequency Resolved Optical Gating (FROG) is a widely used method of characterizing ultrashort pulses in which the pulse's intensity and phase can be extracted from a spectrally resolved auto or cross correlation based on almost any nonlinear optical interaction. Here we are developing a novel FROG approach designed specifically for measuring relatively intense, deep (<300 nm) or extreme (<100 nm) UV pulses which are out of the range of typical silicon detectors. Our approach is similar to Transient Grating (TG) FROG in that a grating is formed by interfering a pair of identical UV pulses and a visible or near infrared (near-IR) pulse is diffracted off this grating. In standard TG FROGs, the pulse diffracting off the grating is delayed in time with respect to the other two pulses and the spectrum of the diffracted signal is recorded at each delay. This yields intensity and phase information about the diffracting pulse. In our case however, we scan the delay of one of the UV pulses with respect to the other two, while still measuring the diffracted signal's spectrum at each delay. Delaying the UV pulse instead should provide intensity and phase information about the UV pulses making up the grating.

Here, we present initial tests of this new type of FROG using two 400 nm pulses to make the grating and diffracting an 800 nm pulse.



**Jacob LaMountain**

Program: UGS/Postbac  
School: University of Massachusetts Lowell  
Group: C-NR  
Mentor: Gencho Rusev

Category: Physics  
Type: Individual  
LA-UR: 19-27023

**Neutron-Capture Cross Section from Ir-193**

Accurate measurement of neutron fluence is necessary in evaluating the performance of fissioning devices such as subcritical assemblies, nuclear reactors, and nuclear weapons. Iridium is an important radiochemical detector due to its long-lived isotopes produced via neutron- activation. A few neutron-induced reactions cause the stable iridium isotopes, Ir-191 and Ir-193, to transmute to other short-lived isotopes depending on the incident neutron energy. In particular, the neutron-capture reaction is sensitive to neutrons with energies below 1 MeV. To improve the accuracy of iridium radiochemical measurements the neutron capture cross sections of these reactions must be well known. We performed a measurement of the  $^{191}\text{Ir}(n,\gamma)$  reaction with the Detector for Advance Neutron Capture Experiments (DANCE) at the Los Alamos Neutron Science Center. DANCE is a gamma-ray calorimeter composed of 160 high-efficiency BaF<sub>2</sub> detectors covering a total solid angle of about  $3.6\pi$  which can provide accurate measurement of the total gamma-ray energy released by the neutron-capture reactions. Preliminary results from the analysis of the collected data will be presented.

**Scott Luedtke**

Program: GRA/Post Masters  
School: University of Texas at Austin  
Group: XCP-6  
Mentor: Lin Yin

Category: Physics  
Type: Individual  
LA-UR: 19-25812

## **Predicting QED Photon Jets from Plasma Experiments with Present-Day Lasers**

Discovery of quantum radiation dynamics in high-intensity laser-plasma interactions and engineering new laser-driven high-energy particle sources require accurate and robust predictions. Using QED-particle-in-cell simulations, we investigate a characteristic dipole pattern of high-energy photon emission that results when the laser pulse bores through the target, forming a channel that enhances the laser field. We observe significant stochasticity in macroscopically identical simulations and show that the stochasticity is physical in nature and expected to be present in experiments. The non-deterministic nature of the channeling phenomenon has important implications for designing an experimental campaign to detect QED photons and validate quantum radiation models, namely, experiments must produce a distribution of results to compare with predictions. We explore several ways that experiments differ from most simulations. Based on historical shot data from a petawatt-class laser, we run several simulations and predict the results and variability expected in experiments.

## **Colin Maez**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: P-23

Mentor: Dana Duke

Category: Physics

Type: Individual

LA-UR: 19-26896

## **Digital Holography Microscopy**

Ultraviolet holographic on-axis Fraunhofer holography is a useful tool to characterize ejecta particle size distributions in small scale explosions. On-axis holograms were used to digitally reconstruct image-planes for a three-dimensional image of ejecta experiment. The digital reconstruction was accomplished by applying the Angular Spectrum Method (ASM), where the propagation of a complex wave field is described by the infinite sum of plane waves. This method avoids approximating the diffraction waves, requires smaller propagation distances, provides quicker computational times when compared to the analytical approach, and is more intuitive than other methods (i.e., Fresnel Approximation, Fraunhofer Diffraction, and Huygens Convolution Method). This project implements a faster method to record the reconstruction plane and will replace the current laser scanning system. The digital reconstruction method will then be compared to laser scanned holograms.

## **Joshua Martin**

Program: GRA/Post Masters  
School: Ohio State University  
Group: M-9  
Mentor: Blake Surtevant

Category: Physics  
Type: Individual  
LA-UR: 19-26128

## **High-Precision Equation of State Measurements Using Microfabricated Materials**

Equations of state (EOS) are a necessary tool when modeling material behavior at extreme pressure-temperature conditions on the micro-, meso-, and macro-scales. Although advances in high-pressure, high-temperature experimental capabilities have increased accessible pressure and temperature ranges, EOS must still be extrapolated beyond the range of the experiment. In Earth and planetary sciences, EOS are used to model the structure and evolution of planetary interiors. Extrapolations of the uncertainties in EOS parameters to pressure and temperature conditions relevant to planetary interiors affect the precision with which we can draw quantitative conclusions on the composition and structure of a planet. We report the results of synchrotron-based laser-heated diamond-anvil cell (LHDAC) experiments using mass-produced micro-fabricated samples consisting of sub-micron-thick layers of Fe, MgO, and Fe designed to reduce temperature gradients and retain consistency of sample geometry between experiments. This sample design, combined with a Monte Carlo fitting routine that propagates uncertainty in both the dependent and independent parameters, yields a high-precision EOS for hcp iron, a material relevant to planetary cores. This will serve as a benchmark for future LHDAC experiments conducted with these samples at different synchrotron beamlines, identifying potential sources of uncertainty when comparing experiments across various facilities.

## **Emily Mendoza**

Program: UGS/Postbac

School: New Mexico Highlands University

Group: P-23

Mentor: Verena Geppert-Kleinrath

Category: Physics

Type: Individual

LA-UR: 19-26874

### **MCNP6 Simulations of Neutron Imaging through a Ring Aperture**

Neutron imaging is an important diagnostic tool in understanding the implosion conditions of Inertial Confinement Fusion (ICF) targets. ICF is the compression of a DT (deuterium tritium) capsule using laser drive with the goal of achieving ignition. The CEA, the LLE and the Advanced Imaging Team collaborated to conduct an experiment at the OMEGA facility to evaluate the feasibility of neutron imaging of cryogenic targets. The CEA annulus aperture [1] is composed of tungsten with a penumbral-like hole in the center and a tapered piece of tungsten inserted to form a ring [2]. The ring aperture recovers spatial information from the source similar to a penumbral aperture. The resulting experimental images from the ring aperture, used in the OMEGA experiments initially indicated an asymmetric neutron distribution. A simulation developed with Monte Carlo Neutron and Photon (MCNP6) code was used to study the image formation through the annulus aperture. The simulation consists of both point and distributed neutron sources shifted on and off the axis to test the accuracy of the aperture when misaligned. Using the simulation in comparison to the reconstructed shot data, the effects of alignment, manufacturing accuracy, and source distribution are deconvolved.

**Khanh Nguyen**

Program: GRA/Post Masters  
School: University of Rochester  
Group: XCP-6  
Mentor: Lin Yin

Category: Physics  
Type: Individual  
LA-UR: 19-26033

## **Simulations Study of Nonlinear Saturation of Cross Beam Energy Transfer in TOP9 Experiments at the Omega Laser Facility**

In laser-based inertial confinement fusion (ICF), an ensemble of high energy laser beams drives the implosion of a capsule containing nuclear fuel. Ablation of the capsule surface, however, forms a plasma corona apt for laser-plasma instabilities that can limit the performance of the implosion. Among these instabilities, cross beam energy transfer (CBET), or the exchange of energy between overlapped beams mediated by ponderomotively excited ion-acoustic waves, can scatter light away from the capsule surface. At the Laboratory for Laser Energetics (LLE), an experimental platform, TOP9, has been developed for focused studies of CBET in ignition relevant plasmas. These experiments will establish the limits of linear theory, but an understanding of how CBET saturates at these limits requires detailed simulations. Here we will present the results of VPIC particle-in-cell simulations exploring mechanisms for CBET saturation.

## **Emily O'Donnell**

Program: UGS/Postbac  
School: Rensselaer Polytechnic Institute  
Group: XCP-5  
Mentor: Kevin Honnell

Category: Physics  
Type: Individual  
LA-UR: 19-23901

### **Improving Equation-of-State Performance in xRage**

When performing high-fidelity multiphysics simulations of dynamic phenomena, a significant amount of computational time can be consumed in retrieving thermodynamic data from tabular equation-of-state (EOS) databases. This research investigates two potential ways of reducing this time without compromising accuracy: by “pre-inverting” EOS tables to use density and internal energy, rather than density and temperature, as the lookup variables; and by densifying the EOS tables to allow use of a fast linear interpolation algorithm rather than the slower, rational-function interpolator. Using the LANL hydro code xRage as a testbed, the compressible “dblast” problem was examined with air and deuterium tabular EOSs. When linear interpolation was used and when the rational interpolator was coupled with the `invert_at_setup` option, the runtime was reduced to approximately 50% that of the reference simulation time. When using linear interpolation, the density of the EOS table does not show any significant effect on the timing of the simulation and it was possible to improve the accuracy of the simulation by about twice that of the original, sparse EOS table.”

## Dean Price

Program: UGS/Postbac

School: University of Illinois at Urbana-Champaign

Group: XCP-3

Mentor: James Hill

Category: Physics

Type: Individual

LA-UR: 19-26443

### **1-D P<sub>n</sub> Method for the Radiation Transport Equation**

Radiation transport has a variety of applications from astrophysics to radiation therapy. One method for solving the radiation transport equation involves representing the solution to the equation as a summation of spherical harmonics; this method is known as a P<sub>n</sub> method. This representation allows for the angular dependency of the radiation field to be accounted for without any imposed discretization. Instead, the error in this method comes from truncating the spherical harmonic representation of solution with a finite number of spherical harmonics. This project involves writing a P<sub>n</sub> solver called hyPnos into an existing framework in the RISTRA project. This solver is applied to a few test problems and compared to existing radiation transport solvers. There is already a first order P<sub>1</sub> solver in RISTRA, hyPnos is intended to be extendable to a general order. Thus far, hyPnos is intended to be kept in 1D with a single energy group, this will reduce the complexity of the problem.

The simplest test problem explored is an isotropic source placed at the origin in an initially nonenergetic medium in a cartesian geometry. For this problem, results from hyPnos are compared to results from another established code and some agreement is found. Another test problem explored is the Su and Olson test problem. This test problem is intended to test a reflective boundary condition with a distributed source within the medium. Results from hyPnos are compared to those of another code. Also, the runtimes between existing and new methods are performed.



## **Mohira Rassel**

Program: UGS/Postbac

School: University of Colorado Boulder

Group: T-CNLS

Mentor: Nicole Lloyd-Ronning

Category: Physics

Type: Individual

LA-UR: 19-26328

## **Kilonova Emission - Particle-In-Cell Simulations of Mildly Relativistic Outflows**

One of the unsolved problems in high energy astrophysics is the relationship between amplification of magnetic fields and the process of particle acceleration. The aim of this project is to implement VPIC (vector particle-in-cell) kinetic simulations for collisionless plasma for mildly-relativistic shock simulations over range of parameters including kilonova outflows. Effects of various plasma conditions were observed in magnetic fields and particle energies. Additionally, validity of using different and often unrealistic proton to electron mass ratios in VPIC simulations was tested.

## **Christopher Roper**

Program: GRA/Post Masters  
School: Georgia Institute of Technology  
Group: P-24  
Mentor: Samuel Langendorf

Category: Physics  
Type: Individual  
LA-UR: 19-26082

### **What are the limits to $j \times B$ acceleration of quasineutral plasmas?**

Plasmas can be effectively accelerated using the Lorentz  $j \times B$  force, in configurations such as Marshall guns, railguns, and magnetoplasmadynamic thrusters. These devices have achieved moderate efficiencies  $\sim 20\%$  and high velocities  $\sim 100$  km/s in pulsed operation. Many physical mechanisms exist which can limit the achieved velocity in such a plasma accelerator, including mass addition due to erosion or desorption from the walls, aerodynamic drag forces, or the occurrence of secondary restrike arcs leading to loss of accelerating current in the primary plasma. We explore these mechanisms in the present research and seek to design and develop a plasma railgun with as high a velocity as possible.

**Ian Ruh**

Program: UGS/Postbac

School: University of Wisconsin Madison

Group: T-2

Mentor: Hui Li

Category: Physics

Type: Individual

LA-UR: 19-26959

## **Exploring A New Astrophysical Gas Dynamical Instability on GPUs**

The Kelvin-Helmholtz instability (KHI) is a classic hydrodynamics problem that has been studied extensively. The instability arises when two smooth flows of different velocity interact at a perturbed boundary, ultimately resulting in turbulent flow. In our study we look at a modified setup of the Kelvin-Helmholtz instability where instead of just 1 set of shearing slabs with different densities, there are two sets. This setup serves a local model for astrophysical environments with adjacent filamentary structures, e.g. supernova remnants or ISM clouds. It was recently pointed out that in addition to KHI, there is an independent dynamical instability that will cause the denser slabs to coalesce. In our study we examine the interaction of KHI and 'cloud coalescence'. In particular, we assess whether or not a time varying radiation flux can speed up the coalescence process, so that it occurs on dynamical time scales, thereby competing with KHI. In order to perform the study, we modified a public GPU accelerated hydrodynamics code (Cholla) to include thermal conduction, allowing us to self-consistently model the interfaces between the hot and cold gas phases.

## **Opale Schappert**

Program: UGS/Postbac

School: New Mexico Institute of Mining and Technology

Group: NEN-1

Mentor: Andrea Favalli

Category: Physics

Type: Individual

LA-UR: 19-27029

## **MCNP Simulations of Neutron Fluxes Through Trinity Supercomputer Nodes**

The elevation of the Trinity Supercomputer at Los Alamos National Laboratory poses a unique yet significant challenge; the effects of cosmic rays, specifically the neutrons present in these showers, have a chance of inducing soft errors in the memory of the supercomputer. These errors pose a major concern in reliability, as they can corrupt or interrupt calculations. Depending on their energy, neutrons can induce reactions in semiconductors and doping materials, which in turn produce charged particles that, by ionizing locally, can generate soft errors in the memory of a supercomputer. Fast neutrons, for example, can produce  $^{28}\text{Si}(n,\alpha)^{25}\text{Mg}$  (Threshold 2.75 MeV) or  $^{28}\text{Si}(n,p)^{28}\text{Al}$  (Threshold 4 MeV) nuclear reactions, while thermal neutrons (energy less than 0.5 eV, the Cd cut off energy) produce  $^{10}\text{B}(n,\alpha)^7\text{Li}$  reaction which features a very high cross section.

To address and explore the impact that neutrons of different energies can have on the Trinity supercomputer, we developed a comprehensive model of the situation. Using MCNP 6.2 Monte Carlo code, we built a detailed model of the Trinity Supercomputer to run simulations focused on terrestrial neutron distribution. The model contains the full environment of the Trinity racks, which includes the floor, the cooling systems, and the surrounding materials, all of which are necessary for the fidelity of the simulation. Multiple simulations were performed in 3 neutron energy groups: 0-0.5 eV, 0.5 eV - 1 MeV, 1 MeV - 15 MeV, and the distributions in the supercomputer nodes were calculated. These simulations show which nodes of the Trinity racks that depending on the energy of the neutrons, are most likely to be affected by neutron induced reactions and can help us find ways to circumvent these issues.

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## Rachel Sidebottom

Program: UGS/Postbac  
School: Occidental College  
Group: E-6  
Mentor: Michelle Espy

Category: Physics  
Type: Individual  
LA-UR: 19-25892

### **Au-leaf phantoms of Au-tagged tumors to assess proton radiography for image-guided proton therapy**

Rachel Sidebottom, Dale Tupa, Matthew Freeman, Per Magnelind, Frank Merrill, Michelle Espy

Proton therapy is a well-established method of cancer treatment, with a demonstrated improvement in outcomes due to dose reduction in sensitive tissues that reduce treatment-related side effects. Relativistic (~1 GeV) protons have the potential to provide more precise, submillimeter, treatment of tumors than the typical proton energy of 230 MeV currently widely in use. However, in order to take advantage of sub-mm precision in dose delivery, a real-time in-place imaging capability is needed to guide the treatment, to account for real-time changes in organ motion and anatomical alignment. Relativistic proton radiography is an enabling technology for this advance in proton beam therapy. Here, Au-leaf phantoms were developed to assess the resolution and quality of proton radiographs made at the Los Alamos Proton Radiography Facility (pRad) for the application of image-guided proton beam therapy for cancer. These phantoms, based on calculations which correlate a given thickness of gold to scenarios for tagging cancers with gold nanoparticles (AuNPs), consist of gold leaf placed on an acrylic backing. The calculations display which phantoms best describe particular tagging scenarios, and are also applicable to phantoms made by injecting AuNPs into a mouse model. The phantoms created were imaged to optimize the configuration of the pRad beamline and our data analysis techniques, to determine the radiation dose needed for an image adequate to guide proton beam therapy, and to confirm our calculations of the image resolution that we expect. Using a x7 proton magnifying lens with the 800-MeV LANSCE proton beam, a 1- $\mu\text{m}$ -thick Au foil was visible, representing a material percent density change of 0.2%, indicating that this proton radiography technology could be applicable to characterizing smaller tumors, and thus allowing for earlier treatment and detection of cancer.

## **Landon Tafoya**

Program: UGS/Postbac

School: Washington University in St. Louis

Group: P-23

Mentor: Verena Geppert-Kleinrath

Category: Physics

Type: Individual

LA-UR: 19-26883

## **A Dense Plasma Focus as a Potential Source for Neutron Radiography**

Co-Authors: Carl Wilde, Matt Freeman, Josh Tybo, Jason Allison

A dense plasma focus (DPF) device electromagnetically accelerates and condenses ionized gas (plasma) to the point of nuclear fusion, producing an intense beam of ionizing radiation (primarily 14 MeV neutrons and x-rays). As such, a DPF device has the potential to be used as a neutron source for radiography, which requires a point-like source for high resolution images. To assess the feasibility of a DPF for this application, the source size was measured experimentally using a neutron imaging system, given that the (magnified) source size can be obtained from a neutron image by de-convolving the detector blur from the source blur. The experimental setup consists of a DPF device positioned in front of collimation that creates a 20 cm window for rolled edge test apertures. A rolled edge aperture with a radius ensures the image contains an edge to determine resolution regardless of misalignment with the source. Produced neutrons travel through the rolled edge aperture, to a 4 cm thick plastic scintillator, where produced light is collected by a lens onto a Photek S25 MCP II Image Intensifier and a SI-800 CCD camera. The source size is obtained from analysis of shot data from a recent DPF campaign at the Nevada National Security Site, which defines the feasibility of using a DPF device for future neutron radiography diagnostics in subcritical experiments.

**Alisha Vira**

Program: UGS/Postbac

School: Smith College

Group: ISR-1

Mentor: Philip Fernandes

Category: Physics

Type: Individual

LA-UR: 19-26736

## **Solid-State Detectors: A Novel Space Mass Spectroscopy Technique**

Space plasma mass spectrometry commonly uses carbon foil-based or linear electric field time-of-flight instruments to characterize magnetospheric ions (e.g. Van Allen Probes/HOPE at Earth, Cassini CAPS at Saturn, etc.). However, the Z- plasma spectrometer (ZPS) aboard the Space and Atmospheric Burst Reporting System (SABRS) payload uses a novel mass spectrometry technique to differentiate between common species in Earth's inner magnetosphere, like H<sup>+</sup> and O<sup>+</sup> ions. This low-resource technique exploits the energy loss of ions in solid-state detectors (SSDs), enabling low-resource mass spectrometry with no additional instrument complexity. The instrument consists of an electrostatic analyser, which selects the energy-per-charge of the incoming ions, and a silicon solid-state detector. We present the modelled output signal from the SSD for H<sup>+</sup> and O<sup>+</sup> ions using the Monte-Carlo software SRIM (stopping range of ions in matter) to understand the physics of this mass spectrometry technique. We find that at low energies ( $\leq 150$  keV) the separation between H<sup>+</sup> and O<sup>+</sup> peaks is driven by the nuclear stopping defect, an intrinsic property of solid-state detectors; at high energies ( $> 150$  keV), the peak separation primarily is driven by the energy straggling through the inactive layer. We compare the modelled and instrument pulse height distributions and find remarkable agreement between the two distributions. We then characterize the instrument response to show that we can distinguish H<sup>+</sup> and O<sup>+</sup> ions at a range of energies.

## **Braden Weight**

Program: GRA/Post Masters

School: North Dakota State University

Group: T-1

Mentor: Sergei Tretiak

Category: Physics

Type: Individual

LA-UR: 19-26042

### **Defect Concentration and Configuration Dependence on Optical Features in Carbon Nanotubes**

Carbon nanotubes (CNTs) have been recently studied in more depth due to their promise of superior electronic properties for purposes of tunable emission in the infrared. Optical features of functionalized carbon nanotubes have been narrowed to only a few main parameters: (1) chirality, (2) defect configuration, and (3) defect electronegativity. Until recently, no literature has shown the effects of defect concentration on carbon nanotubes. Previous theoretical studies have been directed at single-defect pairs attached to the carbon nanotube surface, and these pairs give a wide range of tunability toward emission features, but in the same recent literature, only some defect configurations have shown to be more thermodynamically and kinetically stable. More importantly, it has been suggested that one defect configuration may direct the next, nearby defect attachment toward a different configuration. Experimental spectra at varying concentrations show broad peaks at energies not well matching with a single attachment that may be composed of multiple varying attachments. In this work, using density functional theory (DFT) and time-dependent DFT (TD-DFT), we show defect concentration dependence on the excited state properties of CNTs. We explore redshifts in the lowest, bright transition to flesh out the interactions between the defects and relate these trends to the well-known and simple HJ-aggregate exciton theory. In addition, we explore the thermodynamic stability of these species by comparing relative energies.



## Calvin Young

Program: UGS/Postbac

School: University of Missouri - Columbia

Group: P-24

Mentor: Eric Loomis

Category: Physics

Type: Individual

LA-UR: 19-26991

### **Effects of Asymmetries on the Evolution of an Indirectly Driven ICF Capsule Outer Shell**

Nuclear fusion offers the possibility of clean power production in a compact form, and as such is a focus of many different avenues of research. Inertial Confinement Fusion (ICF) is particularly promising, although many hurdles remain in the attainment of fusion experimentally. Indirectly driven ICF methods involve a spherical capsule placed inside a high-Z (e.g., Au) metallic chamber (hohlraum). Capsules are composed of deuterium-tritium fuel sheathed in one or more layers (shells) of specially selected materials. Lasers are pulsed into the hohlraum, ablating the metal walls, and bathing the capsule in x-rays, ablating the outer shell of the capsule. The ionized outer shell is forced inwards by the ablative force, compressing the inner layers like a pusher/piston, until the fuel reaches an energy state at which robust burning and fusion reactions may occur. A configuration of two shells with spacers, or a Double Shell, offers particular advantages such as energy retention and stability. Fabrication of the shells in this method is difficult, however, and the resultant form may be an imperfect spheroidal shape. These imperfections lead to deflection and asymmetrical evolution as the outer shell implodes from ablative force, introducing instabilities which can reduce compressive efficiency. It is thus necessary to be able to characterize the shape of the outer shell before an experiment, in order to predict with simulation the effect of surface deformities and asymmetries on evolution during implosion. I have developed a tool which reads manufacturer profile data of the capsule surface and returns the orientation and spherical harmonics, or characteristic shape data. I then implemented an ablative rocket model in order to characterize the development of shell features during the initial implosion. Further progress will involve calculating the growth spectrum of perturbations based on the initial shape of the shell and data from our implosion model.

## **Trip Haynes**

Program: UGS/Postbac  
School: New Mexico Tech University  
Group: W-10  
Mentor: Jonathan Mace, Francis Martinez

## **Liam Pocher**

Program: UGS/Postbac  
School: Colorado School of Mines  
Group: W-10  
Mentor: Jonathan Mace

## **John Rose**

Program: GRA/Post Masters  
School: Colorado School of Mines  
Group: W-10  
Mentor: Jonathan Mace

Category: Physics  
Type: Group  
LA-UR: 19-26381

## **Understanding Electrostatic Discharge**

In order to better understand threshold electrostatic discharge (ESD) events, the team is working on coupling two different codes to simulate hydrodynamic flow about the discharge channel. This is important when considering high inductance discharge circuits, since the timescale associated with such events is on the order of shock propagation timescales in air. One code is COMSOL Multiphysics, a very capable and robust Eulerian code utilized to simulate the plasma physics/chemistry of the discharge channel (typically over short timescales), thus providing thermodynamic state along the axis of symmetry. The other is a high-order LANL code called CERCION that uses Lagrangian mesh styles to simulate sub/supersonic wave motion outward from the symmetry axis, thus yielding reduced density and increased electron mean free path (mfp) in the discharge channel. Hence, the discharge channel is treated as a source term that drives non-ionizing hydrodynamic flow, and the hydrodynamic flow, in turn effects mfp, and thus plasma physics/chemistry in the discharge channel, and therefore these codes must be iteratively coupled in space and time.

## **Chandler Smith**

Program: UGS/Postbac

School: Occidental College

Group: NEN-1

Mentor: Mark Croce

## **Aidan Tollefson**

Program: UGS/Postbac

School: Bethel University

Group: NEN-1

Mentor: Mark Croce

Category: Physics

Type: Group

LA-UR: 19-26755

## **Decay Energy Spectroscopy of Actinium Isotopes using Transition Edge Sensor Microcalorimeters**

Ac-225 is a potentially valuable medical isotope for targeted alpha therapy in cancer patients and is currently in human trials. However, the synthesis of Ac-225 yields the byproduct Ac-227, which is harmful due to its long half-life. Sufficient detector sensitivity is critical for determining the relative amounts of Ac-225 and Ac-227 in a nuclear medicine sample. Superconducting Transition Edge Sensor (TES) microcalorimeters offer high resolution energy spectroscopy by utilizing the normal-superconducting phase transition to measure small changes in temperature. By embedding alpha-emitting radioisotopes in a gold foil thermally coupled to a TES microcalorimeter, we can maximize the detector efficiency to  $4\pi$  and measure the decay energies of radioactive elements by thermalizing the released energy. This technique simplifies several peaks from alpha decays into single Q-value peaks, disregarding pileup and escape. This highly efficient technique will aid the medical campaign against cancer by providing confirmation of clean Ac-225 doses.

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