# Los Alamos National Laboratory

"Championing Scientific Careers"
Highlighting Student Research

# 15th Annual Student Symposium Abstracts

**August 4, 2015**
**UNM-LA**

Los Alamos
NATIONAL LABORATORY
EST. 1943

# Table of Contents

Index by Category, Student Name

## Biosciences

## Chemistry

# Computing

# Earth & Space Sciences

## Engineering

## Health & Safety

## Information Technology

# Materials Science

Ximone Willis Page 125
*3D Printed Cryogenic Probes for High Magnetic Fields*

## Mathematics

## Non-Technical

# Other

## Physics

**Name:** Ryan Agh

**Program:** UGS/Postbacc

**School:** Belmont University

**Group:** B-11

**Mentor:** Silks, Pete

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-24946

# Synthesis of Unnatural Amino Acids and their Use in Characterization of Proteins

During the last several decades the preparation of selenomethionine- (SeMet) containing proteins has proved to be a valuable tool in the elucidation of three dimensional structure by multiwavelength anomalous diffraction (MAD) techniques. Furthermore, Se-77 NMR spectroscopy has been shown to be an important probe of enzyme structure and function. It is evident that analogs of amino acids that occur at low natural abundance in proteins, such as L-methionine and L-tryptophan, are excellent tools for protein characterization since their contribution to structural and catalytic activities are usually minimal. The potential utility of a selenium-containing tryptophan analog, β-selenolo[3,2-b]pyrrolyl-L-alanine ([4,5]SeTrp), has already been demonstrated in the literature. This finding shows promise for the bio-incorporation of its positional isomer, β-selenolo[2,3-b]pyrrolyl-L-alanine ([6,7]SeTrp), as well as, the tellurium-containing analog, [6,7]TeTrp. The resulting compounds will add to the toolbox of heavy atom-containing amino acids for use in the characterization of proteins. The progress towards the synthesis of [6,7]SeTrp and [6,7]TeTrp will be presented.

**Name:** Ayesha Arefin

**Program:** GRA

**School:** University of New Mexico

**Group:** B-10

**Mentor:** Iyer, Rashi S

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** 15-24567

# Fabrication of Flexible and Thin PU Membrane for Constructing Artificial Alveoli

The current challenge to study lung disease or screen lung drugs requires a reliable in vitro lung model. Recently, microfluidic technology comprising of stacked micro channel networks has been explored to fabricate artificial lungs. However, existing membranes used to impose cyclic stress are limited either by the lack of biocompatibility or the necessary strain profile. Commonly used polymers to fabricate these membranes such as Polydimethylsiloxane (PDMS) have been reported to cause undesired effects such as absorption of small molecules and limited compatibility with large scale production. To address these limitations, we are investigating the application of Polyurethane (PU) to develop thin, flexible, and biocompatible membranes. PU is well known for applications in various biomedical devices and has been shown to cause minimal absorption of small molecules compared to PDMS. We are studying different types of PU including GSP 1552-2 (G.S. Polymers, Inc.) and Bayhydrol (Bayer Material Science). Optically transparent membranes with thicknesses ranging from 6 µm to 20 µm were fabricated using spin coating on silicon and polymeric substrates. We report a unique technique to reproducibly release the membranes form the substrates and mount them on a frame for device integration. The membranes were characterized for their elastic properties using a microfluidic based bulging test system. It is possible to apply up to 6 kPa fluidic pressures to execute cyclic stress on 2 mm diameter membranes without failure. Adenocarcinomic human alveolar basal epithelial cells (A549) and Human microvascular endothelial cell (HMVEC) were co-cultured on the apical and basal sides of the PU membrane, respectively. The morphology and the viability of the cells were compared to cells cultured on standard tissue-culture plates. Our experiments suggest that stretchable PU membrane has potential use for various tissue culture applications including the development of in vitro models of the alveoli.

**Name:** Kirill Balatsky

**Program:** UGS/Postbacc

**School:** University of Colorado at Boulder

**Group:** B-11

**Mentor:** Iyer, Rashi S

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25513

# Protein Composition of Extra Cellular Matrix Effects Tissue Differentiation

Extra cellular matrix (ECM) is an assortment of proteins and molecules secreted by cells into their immediate environment that functions to maintain cell adherence, support, and differentiation. Its composition has a profound effect on cellular adherence and differentiation. This project was primarily concerned with ECM makeup of human bronchial tissue, which consists of collagen, fibronectin, and laminin in a mixture which can vary in healthy and disease states. Markers of healthy differentiation in bronchial cells are tight junction formation, ciliary cell formation and function, mucin production, and pseudostratified epithelial formation. Human bronchial epithelial cells were seeded on transwell culture inserts coated with various ECM proteins alone and in mixtures, differentiated, then cultured for 21 days. Trans Epithelial Electrical Resistance (TEER) is created when tight junctions form between cells. TEER readings were taken twice a week with washes to monitor growth. Light microscopy was done for daily monitoring and imaging. Cells were stained for cilia, actin and nuclei. Image analysis was performed for total cell number, percent ciliated cells, and cilia coverage by area for all experimental ECM trials. Results show that cell growth was best in control and collagen alone samples. While various mixtures of ECM proteins were tested, results were inconclusive towards finding an ideal ratio for ciliary differentiation.

**Name:** Charlotte Berg

**Program:** UGS/Postbacc

**School:** Smith College

**Group:** MPA-CINT

**Mentor:** Omberg, Kristin Marie

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25188

# Long-Term Storage of Antigens in Silica Sol Gels

A proof-of-principle experiment was performed to determine whether Yersinia pestis F1 antigen remains stable when stored in silica sol-gels at room temperature for extended periods of time. The F1 antigen is a protein found on the surface of Yersinia pestis capsules. Clinics and researchers use the F1 antigen to detect the presence of Yersinia pestis in humans and the environment. Simple lateral flow immunoassays exist that can detect antigens at less than 1 nanogram per milliliter of solution. However, current protocols require the antigen to be stored at extremely low temperatures (-80 C). Using silica gel technology, we are storing F1 antigen (recombinant antigen generated in E. coli) at room temperature. The silica sol gel is created by hydrolyzing tetramethyl orthosilicate (TMOS) and PCR-grade water in a commercial microwave. Excess methanol is evaporated off and antigen is added to form a soft gel defined by multiple silicon-oxygen bonds. Water molecules remain present in the gel matrix. Vortexing disrupts the gel and allows for the liquid sample to be run through an immunoassay or similar test. This could impact clinical storage and has the potential to help testing in locations with little access to clinical resources.

**Name:** Ashley Brooks

**Program:** UGS/Postbacc

**School:** Florida Agricultural & Mechanical University

**Group:** B-11

**Mentor:** Silks, Pete

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-24980

# Bioenergy Concepts Reduced to Practice

Biomass, if efficiently converted to high energy density fuel, has the potential to become a sustainable source of this commodity, instead of petroleum. Biomass is living or recently dead biological material that can be used as fuel. Examples of biomass include corn stover, switch grass, wood chips, and grass clippings. In order for biomass to become a viable fuel source, an efficient process for its conversion into hydrocarbons (i.e. fuel) must be developed. This conversion process has four steps. First, the cellulosic sugars must be extracted from the biomass source. Glucose monomers are extracted from cellulose while arabinose is extracted from hemicelluloses. These sugars are then dehydrated to form critical sourcing materials. Next is a carbon chain extension to give rise to intermediates with the proper length for a fuel. This step is often done using an aldol condensation reaction. Finally, the aldol products are deoxygenated to remove the hydroxyl groups and then hydrogenated in order to yield a hydrocarbon. An example, a very inexpensive 5 carbon unit is levulinic acid and furfural. Combining these affords a 10 carbon unit. Examining new ways to use these units in the carbon-carbon bond forming reactions to give longer carbon chains is the focus of this study.

**Name:** MariJo DeAguero

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** B-11

**Mentor:** Fox, David Thomas Shaw

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25557

# Commodity Chemical Production in Cyanobacteria

Commodity chemicals, such as adipic acid (the building block for nylon 6,6), are produced at large scales from fossil fuels causing negative impacts for the environment. For example, during adipic acid production, teragrams of greenhouse gases are generated and megatons of organic and inorganic waste must be properly—and safely—disposed. An enticing alternative to fossil fuels is exploitation of cyanobacteria (blue-green algae) to biosynthesize the identical intermediates to adipic acid. Photosynthetic cyanobacteria as a renewable carbon source are quite efficient at carbon dioxide fixation, and readily amenable to genetic manipulation. The compound 3-dehydroshikimate (DHS) is part of the metabolic pathway leading to the biosynthesis of aromatic amino acids and a suitable route to generate adipic acid precursors using metabolic engineering platforms. Our team recently discovered a gene, asbF, which creates a shunt pathway by directly converting DHS to 3,4 dihydroxybenzoate (DHB). This engineered pathway serves as the first step toward biobased adipic acid production or for direct use as a food preservative. My role is to introduce this new metabolic pathway into cyanobacteria. This will be accomplished by introducing the foreign DNA, asbF, into the marine cyanobacterium host Synechococcus elongatus sp. strain PCC7002. From there, I will test if there is any enzyme activity in the cyanobacteria. Two mutants of AsbF will also be introduced into PCC7002 through the same process. The first is a null mutant, my negative control, which has previously been altered to prevent DHB from being produced. The second mutant has been altered to be more heat stable, thus increasing “shelf-life” and, hopefully, leading to an increase in DHB production through the shunt pathway. This would represent the first example of commodity chemical production in cyanobacteria and possibly be a pioneering strategy toward downstream production of bionylon in an ecofriendly manner.

**Name:** Samantha Erwin

**Program:** GRA

**School:** Virginia Tech

**Group:** T-CNLS

**Mentor:** Perelson, Alan S

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** 15-25291

## Dynamics of HIV-1 following Infusion of an Anti-HIV Monoclonal Antibody in Vivo

Monoclonal antibodies against HIV-1 are able to act in many different ways in vivo: they can block viral entry, clear plasma virions or lead to the death of virus-expressing cells. We hypothesize that one or a combination of these effects may lead to different virus dynamics than what is typically observed in patients during combination antiretroviral therapy. To test this, we have developed a new viral dynamic model that incorporates the effects of a specific monoclonal antibody binding to HIV-1 virions and HIV-infected cells expressing HIV envelope protein on their surface. Because broadly neutralizing anti-HIV antibodies do not bind all virions, our model includes a viral strain that is sensitive to the antibody and one that is partially resistant to the antibody. We fit the model to HIV RNA measurements from patients given a monoclonal antibody and we conclude that the presence of the antibody enhances virus clearance explaining an initial decay observed immediately after antibody infusion. Following the initial decay, the HIV-RNA then rebounds. Our model attributes this rebound to the resistant strain that has not yet been cleared. Neutralization of the virus due to the formation of antibody-virus complexes ultimately causes a longer-term decay observed in clinical data. Our model also suggests that productively infected cells are killed by antibody-dependent effects, such as antibody-dependent cellular cytotoxicity (ADCC), starting at approximately two weeks after antibody infusion. In summary, we have provided a comprehensive model that captures the observed effects of monoclonal antibody infusion on the plasma viral load in HIV-infected patients.

**Name:** Andrew Hatch

**Program:** GRA

**School:** University of Southern Maine

**Group:** B-11

**Mentor:** Vuyisich, Momchilo

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25467

# SPIDR-WEB: An Efficient NGS Platform for Diagnostic Applications

We are transforming the field of infectious disease diagnostics with the development of the Sample Prep for Infectious Disease Recognition With EDGE Bioinformatics (SPIDR-WEB) platform that enables efficient use of next generation sequencing (NGS) for pathogen detection in clinical samples. NGS has become a powerful tool for detection and characterization of both known and emerging pathogens. In most clinical samples, the relative abundance of pathogen nucleic acids (DNA or RNA) is vanishingly small. Therefore, vast amounts of sequence data must be generated and analyzed to identify rare pathogen sequences. SPIDR-WEB is a sample-to-result process that relies on efficient laboratory and in silico steps. Clinical samples mostly comprise non-informative host RNAs or abundant housekeeping gene transcripts. SPIDR-WEB incorporates removal of non-informative RNAs (RNR), thereby enriching all other RNAs, including those from pathogens. This step enables either higher sensitivity and specificity, or less expensive and faster sequencing. Our custom EDGE bioinformatics data analysis platform provides rapid read classification at all taxonomic levels, and reliably detects all organisms present in a sample. EDGE is an efficient process, as it uses databases with pre-computed signatures, instead of aligning sequencing reads to the entire Genbank. In addition to RNR and EDGE, SPIDR-WEB includes robust, inexpensive and rapid sample lysis, RNA extraction, and library preparation steps.

**Name:** **Meghan Hill**

**Program:** **UGS/Postbacc**

**School:** **Monte del Sol Charter School**

**Group:** **B-11**

**Mentor:** **Marti-Arbona, Ricardo**

**Category:** **Biosciences**

**Type:** **Individual Poster**

**LA-UR:** **LA-UR-15-25402**

# Discovery of New Drug Targets to Defeat Human Pathogens

Pathogenic bacteria have a remarkable ability to adapt and overcome antimicrobial therapies. With current antibiotics not being effective towards antimicrobial resistant (AMR) bacteria, new methods of inhibiting AMR are desperately needed. Developing a pool of drug targets to respond to the continuous adaptation and evolution of pathogens to antimicrobials is essential to maintain our advantage in the fight against infectious diseases. In this project, we focus in determining new protein targets for pathogens with multiple AMR. We have developed a RNA-based technique that allows the post-transcriptional regulation of protein expression to test whether a protein is essential to either the pathogen's survival or AMR, mimicking antimicrobial effects of antibiotics. We are using Burkholderia thailandensis (Bt), to test synthetic RNA-based regulatory elements (RbREs) that target the AMR mechanism responsible for Gentamycin and Ciprofloxacin resistance. AmrA is a structural component of the efflux pump linked to the Gentamycin resistance in Bt. RecA has been identified as the first mechanism for Ciprofloxacin resistance. Interestingly, we discovered that the AmrAB efflux (responsible for Gentamycin resistance) acts as secondary resistance mechanism for Ciprofloxacin. We have developed RbREs that target AmrA and RecA, inhibiting their expression and restoring the Bt's antibiotic susceptibility to Gentamycin and Ciprofloxacin. Our results validate the utility of the RbREs towards the inactivation of AMR proteins and pave the way for their deployment for the identification and validation of new drug targets against pathogens.

**Name:** Mohammad Ishak

**Program:** GRA

**School:** Tulane University

**Group:** B-11

**Mentor:**

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25466

# In Vitro Evolution of Influenza A Virus Under Artificial Selective Pressure

RNA viruses cause many significant diseases worldwide, such as Dengue and Yellow fevers, the Flu, AIDS, etc. These viruses evolve rapidly and few antiviral therapeutics and vaccines exist. Viral evolution remains poorly understood. We are studying the evolution of RNA viruses under laboratory conditions. Our research aims to answer important questions about the prediction of virus phenotype form its genotype, protein mutations and function, and functions of structural RNAs. We are currently focused on the human Influenza (IAV) virus. Our experimental design creates an artificial environment for viral infection and our hypothesis is that we will be able to direct viral evolution in a specific and desired way. We have engineered host cells (supplemental cells) to express proteins that the IAV naturally produces. After the series of infections of the supplemental cell lines, we will study the effect of this supplementation on the viral evolution. We expect that the viral population will evolve to efficiently infect the supplemental cells and lose the ability to infect the wild type (natural) cells. If our hypothesis is correct, this approach may provide novel viral therapeutic approaches.

**Name:** Maci Joseph

**Program:** UGS/Postbacc

**School:** Howard University

**Group:** B-10

**Mentor:** Gao, Jun

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** 15-25713

# Using Droplet-Based Microfluidics to Perform Digital PCR

The purpose of this research is to encapsulate a single cell inside of a device generated droplet for in-depth analysis. To facilitate the release of nucleic acids within each cell, a lysis buffer solution is symmetrically flown into the device before the droplet is formed. The poly-T conjugated polystyrene beads are co-encapsulated inside of the droplets. Once this is complete, the released RNAs can bind to the beads. Then, the polymerase chain reaction can be conducted on RT-PCR machine or on the chip to quantify the RNA and identify rare sequences. We present a droplet-based microfluidic process that allows for high-throughput screening. Encapsulation of a single cell inside of a droplet enables the analysis and manipulation of the behavior of a single cell when paired with a lysis buffer, probe-conjugated beads or any reagent. Microfluidics is a convenient and low-cost technology that makes generating a large sample size for analysis a time-effective process. By manipulating the cell concentration and flow rates of the continuous and aqueous phases, maximum single-cell encapsulation can be achieved. In the present study, we used a simple flow-focusing device to enclose a single THP 1 or Jurkat T cell with polystyrene beads into water-in-oil droplets.

**Name:** David Li

**Program:** UGS/Postbacc

**School:** UT Austin

**Group:** T-CNLS

**Mentor:** Perelson, Alan S

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25692

# Sensitivity Analysis of Simian Human Immunodeficiency Virus Infection Models

Infecting macaques with simian human immunodeficiency virus (SHIV) provides an excellent model for HIV infection in humans. A recent experimental study was performed to understand the transmissibility and replicative capability of the drug-resistant mutant relative to the wild-type SHIV, in which the dataset shows that the level of viral RNA increasing to an extremely high level (10^5-10^8 copies/mL), then decreasing rapidly to a low level (10^1 to 10^3 copies/mL), and after 15-20 weeks from infection, staying roughly constant. However, viral dynamic models do not describe the primary infection dynamics seen in the dataset well. To explain the pattern seen in the data, we developed multiple new models by incorporating biology of acute infection, such as immune response, abortive infection, and long-lived infected cells. For these models, we statistically evaluated their goodness-of-fit using least-squares regression, and then performed sensitivity analysis by varying individual parameter values to evaluate how well the estimated parameters were constrained by the data. We further calculated the Hessian matrix for the best-fit parameter values to quantify the sensitivity of the goodness-of-fit to multidimensional variations in parameter values. These analyses allow us to assess the reliability of the estimated values and determine the death rate of abortively infected cells.

**Name:** Amanda Mercer

**Program:** UGS/Postbacc

**School:** Whitman College

**Group:** B-11

**Mentor:** Cui, Helen

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25515

# Middle East Respiratory Syndrome Coronavirus (MERS-CoV)

Middle East respiratory syndrome coronavirus (MERS-CoV) is a severe acute respiratory syndrome (SARS)-like virus that affects the respiratory system of patients. Most patients develop severe acute respiratory illness symptoms including: fever, cough, shortness of breath, acute pneumonia, and acute renal failure.[1] In June 1012, the first case of MERS-CoV was reported in a 60-year-old man from Jeddah, Saudi Arabia.[2] As of July 12th, 2015, there have been a total of 1045 laboratory confirmed cases of MERS-CoV infection. About 44% of the confirmed cases have resulted in fatalities. All cases have been linked to countries around the Arabian Peninsula.[3] Like all other coronaviruses that affect humans, MERS-CoV is assumed to have a zoonotic origin.[2] Bats are believed to be the ultimate reservoir of MERS-CoV, but camels also appear to play a role in the transmission of the virus.[4] Humans can be infected by exposure to air, or by consuming infected camel milk or meat.[5] MERS-CoV is not a human virus; it is primarily an animal virus. It is not considered to have pandemic potential because it does not spread easily between humans. MERS mainly spreads in hospital settings and it has been observed that close contact with an infected patient has the potential to transmit the virus.[6] In June 2015, there was an outbreak of MERS-CoV in South Korea. This outbreak was the largest outbreak of the disease outside of the Middle East, infecting 186 individuals, including 36 deaths.[5] The recent outbreak in South Korea brings more urgency to studying this virus and its mechanisms of transmission and pathogenesis. Collaborating with Middle Eastern partners, we sequenced three coronaviral strains and studied the phylogenic relationships. We will present the phylogenic correlation of these strains with other known strains. References: 1. CDC, 2. Utrecht University, 3. Medical News Today, 4. Emerging Infectious Disease Journal, 5. ProMED-mail, 6. Scientific American.

**Name:** Ashley Renfro

**Program:** UGS/Postbacc

**School:** Clark University

**Group:** MPA-CINT

**Mentor:** Omberg, Kristin Marie

**Category:** Biosciences

**Type:** Group Poster

**LA-UR:** LA-UR-15-25179

# Preventing Nosocomial Infections Using Nanostructure Surface Coatings

One out of every twenty patients who walk out of a hospital will have contracted a nosocomial infection from medical devices. Bacteria have the unique ability to grow and colonize in nearly every place in the human body, as long as they have a mechanism to enter. The use of any surgical device that enters the body can result in bacterial colonization at the exit site if not treated with a disinfectant. In phase 1 of our project, we investigated the hypothesis that Graphene, Graphene Oxide, and Silver nanoparticles may possess antimicrobial properties. If this hypothesis is supported, we will work towards developing a permanent antimicrobial coating for invasive devices used to prevent nosocomial infections. We tested various concentrations of the nanoparticles with a representative gram-positive bacterium, B. thuringiensis, as well as a representative gram-negative bacterium, E. coli. Optical density measurements, plating, and SEM microscopy were used to measure both growth and viability of each species and understand structural properties of the nanoparticles, respectively. In phase 1, B. thuringiensis was more susceptible to Graphene, potentially due to cell killing effect. This is seen by the similarity between the growth and viability experiments. The Ag nanoparticles exhibited a greater effect on B.thuringiensis

**Name:** Ambrose Rice

**Program:** UGS/Postbacc

**School:** Belmont University

**Group:** B-11

**Mentor:** Silks, Pete

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-24984

## Synthesis of Unnatural Amino Acids and Bio-incorporation into Selected Proteins

For decades, the use of selenium-containing amino acids, such as seleno-methionine (SeMet), has been the method of choice for specific heavy-atom labeling of proteins for three dimensional structure determinations by NMR spectroscopy, mass spectroscopy, and multi-wavelength anomalous diffraction (MAD) techniques. Unnatural tryptophan analogs containing selenium offer an additional heavy-atom labeling option to aid structural determination of proteins as well as provide new ways to analyze and characterize the function of tryptophan within the active sites of catalytic proteins. Selenium-containing tryptophan analogs can be synthetized enzymatically by coupling the selenolo-pyrrole (indole analog) to serine using Tryptophan Synthase. The utility of the selenium-containing tryptophan analog, 6-(4H-selenolo[3,2-b]pyrrolyl)-L-alanine ([4,5]SeTrp), has been reported in the literature. This shows promise for its positional isomer, 4-(6H-selenolo[2,3-b]pyrrolyl)-L-alanine ([6,7]SeTrp), as well as, the tellurium-containing analog, [6,7]TeTrp, to be successfully bio-incorprated into selected proteins of interest. Progress on the enzymatic syntheses of [6,7]SeTrp and [6,7]TeTrp using tryptophan synthase and their subsequent bio-incorportaion into selected proteins will be presented.

Name: Phillip Stringer

Program: UGS/Postbacc

School: Tuskegee University

Group: B-10

Mentor: Gao, Jun

Category: Biosciences

Type: Individual Poster

LA-UR: 15-25712

## Development of Microfluidic-based Microvalves, Rotary Pump, and Mixer

In recent years interest in microscale chemical reactions and flow control has led to the development of a variety of tools and techniques to elicit gains from the unique properties of materials found at the microscale. For example, one main benefit is reducing reaction times from hours to milliseconds due to shorter diffusion distances and higher surface to volume ratios. Microfluidics as a whole is a multidisciplinary field, which encompasses a range of core principals from areas such as physics, chemical engineering, and biology. We present a review of microfluidic devices used as peristaltic rotary micropumps and micromixers. The objective of this research was to determine the optimal design, fabrication procedure, and operating parameters (e.g. flow rate, pressure, valve open/close sequence) for an easy to use PDMS microfluidic device. An Elveflow OB1 microfluidic flow controller synchronized with an Elveflow Mux microfluidic flow switch matrix was used to pneumatically control microvalve open/close sequences. An algorithm was developed to create a peristaltic pumping effect based on the displacement of fluid within a microchannel. Additionally, this phenomenon was used to mix fluids inside a circular channel. This platform can be integrated with other microfluidic devices to accomplish desired functionalities to improve technologies involving microreactors for catalysis and chemical synthesis, point-of-care diagnostics, drug delivery, cell/molecule compartmentalization and diagnostic testing.

**Name:** Ashvini Vaidya

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** MPA-CINT

**Mentor:** Omberg, Kristin Marie

**Category:** Biosciences

**Type:** Group Poster

**LA-UR:** LA-UR-15-25179

# Preventing Nosocomial Infections Using Nanostructure Surface Coatings

One out of every twenty patients who walk out of a hospital will have contracted a nosocomial infection from medical devices. Bacteria have the unique ability to grow and colonize in nearly every place in the human body, as long as they have a mechanism to enter. The use of any surgical device that enters the body can result in bacterial colonization at the exit site if not treated with a disinfectant. In phase 1 of our project, we investigated the hypothesis that Graphene, Graphene Oxide, and Silver nanoparticles may possess antimicrobial properties. If this hypothesis is supported, we will work towards developing a permanent antimicrobial coating for invasive devices used to prevent nosocomial infections. We tested various concentrations of the nanoparticles with a representative gram-positive bacterium, B. thuringiensis, as well as a representative gram-negative bacterium, E. coli. Optical density measurements, plating, and SEM microscopy were used to measure both growth and viability of each species and understand structural properties of the nanoparticles, respectively. In phase 1, B. thuringiensis was more susceptible to Graphene, potentially due to cell killing effect. This is seen by the similarity between the growth and viability experiments. The Ag nanoparticles exhibited a greater effect on B.thuringiensis

**Name:** Haide Vela-Alvarez

**Program:** UGS/Postbacc

**School:** College of the Desert

**Group:** B-11

**Mentor:** Marti-Arbona, Ricardo

**Category:** Biosciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25401

# Testing of an Algal Fatty Acid Sensing Bioswitch

Microalgae are currently being grown and harvested for biofuel production. Despite their inherent potential as an alternative to fossil fuels, the high cost of growing, harvesting and processing lipid producing algae is impeding the availability of biofuels for commercial use. One of the major contributors is the high costs that arise from the specialized instrumentation required to monitor growth and optimal harvest time. The goal of this project is to develop a bioswitch that senses concentrations of fatty acids within the algae and express a green fluorescent protein in response. Specifically, I will be testing a bioswitch engineered for the model algae organism, STA6-Chlamydomonas reinhardtii (Chlamy). Controlling the expression of the green fluorescent protein (GFP) is FadR, a fatty acid metabolism regulator protein from E. coli. FadR restrains the expression of the GFP by binding to FadO, a DNA operator sequence placed within the promoter used to express the GFP. FadR binds FadO in the absence of long-chained fatty acyl-CoA, once their concentrations increase, FadR releases FadO and allows for the expression of GFP. By creating and validating this bioswitch, we will create a new tool that will allow for the use a fluorimeter to identify when the algae are at their optimal stage of lipid production, and ready for harvesting. Fluorimeters are cheaper compared to the instruments are currently being used and can be deployed to the production fields. This project would reduce the need and cost for expensive instruments, aiding algae biofuels to become more accessible for commercial use.

**Name:** Brian Dolinar

**Program:** GRA

**School:** University of Wisconsin-Madison

**Group:** C-IIAC

**Mentor:** Kozimor, Stosh Anthony

**Category:** Chemistry

**Type:** Individual Poster

**LA-UR:** 15-25950

# Structural and Electronic Characterization of Lewis Acid Activated Mo2 Complexes

Heterotrimetallic complexes of the type Mn+[Mo2]4+ involve a quadruply bonded [Mo2]4+ with a third metal held in the axial position of the Mo2 unit by a bridging ligand, such as 2,2'-dipyridylamine. Previous examples have focused on the formation of Mn+[Mo2]4+ compounds in which Mn+ is a divalent first or second row transition metal. Through the use of the bridging ligand monothiosuccinimide, which contains both a hard base and a soft base, we have greatly expanded the scope of Mn+[Mo2]4+ complexes to include examples in which the heterometal is a member of Groups I, II, and III as well as the lanthanides. The synthesis, structural characterization, and electrochemistry of these compounds are presented here. We also present here the current efforts to extend the scope of these compounds to include actinides (Th and U) as the heterometal.

**Name:** James Jenkins

**Program:** UGS/Postbacc

**School:** Angelo State University

**Group:** C-AAC

**Mentor:** Xu, Ning

**Category:** Chemistry

**Type:** Individual Poster

**LA-UR:** UR-15-25726

# Design and Testing of Centrifugal Microfluidic Devices for Actinide Separation

Microfluidic devices are becoming increasingly popular due to their ability to analyze minute amounts of reactants and their capability to run hundreds to thousands of tests per minute. These "Lab-on-a-chip" devices have been shown to be effective when used for actinide separation. In an effort to make this technology more practical for use in a lab setting, we have designed a centrifugal "Lab-on-a-CD" concept that reduces the amount of equipment needed in a radiologically sensitive area. These devices also allow for the user to perform multiple tests at one time due to the fact that there are 6, 100 µL columns within each device. Our proof-of-concept tests using H2O, show that these devices have the potential to be used for actinide separation.

**Name:** Morgan Kelley

**Program:** GRA

**School:** Washington State University

**Group:** T-1

**Mentor:** Yang, Ping

**Category:** Chemistry

**Type:** Individual Poster

**LA-UR:** 15-25685

# Solvation of Trivalent f-element Ions in Binary Water/Methanol Solutions

Due to their highly ionic character, the trivalent f-element cations impose significant order in polar solvents (for example, water), and their solvation is an important parameter affecting molecular interactions. This is particularly evident in solution complexation reactions, where entropy gains can override enthalpic interactions and cation desolvation is a main thermodynamic driver. While these solvation phenomena have been extensively studied in water, significantly less attention has been paid to mixed solvents – despite their prevalence at D.O.E. waste sites. This work explores differences in ion-solvent binding based on the composition of the primary solvation shell of the trivalent f-element ions using a combination of density functional theory gas-phase calculations, classical molecular dynamics, and ab-initio molecular dynamics.

**Name:** Alexandra Mechler-Hickson

**Program:** UGS/Postbacc

**School:** University of Wisconsin - Madison

**Group:** C-IIAC

**Mentor:** May, Iain

**Category:** Chemistry

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25607

# Development of a Uranium Detection Technique

Mo-99 is a critically important medical isotope used in the vast majority of diagnostic imaging for which no production facility currently exists in the US. The NNSA Office of Material Management and Minimization is partnering with commercial entities in an effort to accelerate the domestic production of Mo-99 without the use of High Enriched Uranium. One such company, SHINE Medical TechnologiesTM, is proposing to use advanced accelerator technology to produce Mo-99 from Low Enriched Uranium (LEU). Their LEU target would be in the form of uranium(VI) sulfate solution, and our challenge has been to develop a specifically tailored method for determination of uranium concentration in such a solution. This method would complement an 'industry standard' technique such as the Davis-Gray titration method. Previous work performed at LANL has led to the development of a UV-vis technique to meet this challenge, utilizing the fact that the uranyl dication (UO22+) absorbs in the visible region with a very distinctive spectroscopic signature. Using this technique, samples can be analyzed quickly and efficiently using small aliquots of solution (uncertainty<1%). Additional experimental measurements have now been performed in order to further validate the use of the UV-vis technique, including reducing uncertainties. Standard solutions with a range of known uranium concentrations were used to recalculate the molar absorptivity of the main peak in an effort to reduce one of the main contributors to the uncertainty budget. Spectroscopic cells from different companies and with different path lengths were evaluated, as was a new method of spectroscopic data collection. Technique development was undertaken using solutions for which accurate density measurements were collected in conjunction with sample mass measurements, thus minimizing errors associated with volumetric measurements. The refined technique has also been tested against 5 'unknown' samples, and the results will be compared with Davis-Gray

**Name:** Julia Murphy

**Program:** UGS/Postbacc

**School:** University of Alabama

**Group:** C-IIAC

**Mentor:** Sutton, Andrew

**Category:** Chemistry

**Type:** Individual Poster

**LA-UR:** 15-25601

## Simple Molecules to Understand Complex Problems

The water-gas shift (WGS) and reverse water-gas shift (RWGS) reactions play important roles in ammonia, hydrocarbon, methanol, and hydrogen manufacturing, as well as in the development of alternative fuels production. These reactions require a heterogeneous catalyst or a Lewis acidic homogeneous catalyst. Lanthanides are good Lewis acids and may be capable of catalyzing the WGS and RWGS reactions. A redox active cerium metal center paired with sterically demanding spectator ligands is a viable candidate for such a catalyst. Through breaking the reaction mechanism into a series of homogeneous intermediates, the reaction can be conducted stepwise by generating the requisite cerium complexes.

**Name:** Belinda Pacheco

**Program:** UGS/Postbacc

**School:** Texas Tech University

**Group:** C-CDE

**Mentor:** Leibman, Chris

**Category:** Chemistry

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25450

## Novel Processing Techniques for Post-Detonation Debris Using Ammonium Bifluoride

Analysis of post-detonation nuclear debris is of critical importance for the elucidation of nuclear device design and of weapon origin. Existing methods for sample preparation of post-detonation material use large quantities of concentrated, hazardous mineral acid fluxes and are lengthy and laborious. A novel approach being considered involves the use of ammonium bifluoride (NH4)HF2 for the dissolution of fused glass samples containing various actinides and fission products. This approach is a more efficient sample processing method for the purpose of rapid actinide isotope ratio analysis compared to conventional techniques. We used thermodynamic modeling software to establish the optimum experimental conditions for the complete digestion of the glassy matrices and the fluorination of actinides, fission products, and other metals using ammonium bifluoride (ABF). In this study, the thermodynamic modeling was applied for the development, exploration, and comparison of various methods for digesting representative glass samples with ABF. The methods considered included microwave assisted digestion, conventional oven, and hot plate supported dissolutions. Quantification of actinides and other metals in National Institute of Standards and Technology standard glass reference materials was performed using ICP-OES and ICP-MS. ABF was seen to provide a significantly faster and safer method for sample preparation and yields quantitative recovery of actinides, fission products and other metals.

**Name:** Danil Smiles

**Program:** GRA

**School:** University of California, Santa Barbara

**Group:** C-IIAC

**Mentor:** Gaunt, Andrew James

**Category:** Chemistry

**Type:** Individual Poster

**LA-UR:** LA-UR-14-25343

# Studies of Actinide Chalcogenide Bonding

Understanding of the structure and bonding of the early to mid transuranic actinide ions provides fundamental chemical knowledge to underpin processes and waste remediation strategies related to Nuclear Fuel Cycles. Exploration of transuranic coordination chemistry under non-aqueous inert atmospheric conditions can inform upon the relevance and extent of covalent interactions. There has been a growing interest in actinide chalcogenides (E = S, Se, Te) due in part to the desire to gain a better understanding of actinide-ligand bonding. My research at UCSB has focused on the developing new methods for installing these functional groups, as well as the synthesis and characterization of these new complexes. While significant work has been done with uranium, the analogous chemistry of the transuranium elements, e.g. neptunium and plutonium, remains underdeveloped by comparison. We are exploring ways to translate the chemistry developed for uranium to that of Np and Pu. New routes towards low valent neptunium starting materials, for these transformations, will also be discussed. My summer research will take advantage of the specialist radiological and material handling facilities at Los Alamos National Laboratory, which are not generally available at a university setting.

**Name:** Nicholas Wozniak

**Program:** GRA

**School:** University of Nevada, Las Vegas

**Group:** C-NR

**Mentor:** Wilkerson, Marianne Perry

**Category:** Chemistry

**Type:** Individual Poster

**LA-UR:** LA-UR-14-28855

# Spectroscopic Signatures for Forensic Sciences

Signatures arising from production, conversion, and aging processes are chemical in nature, and optical measurements reveal the potential to detect persistent molecular signatures characteristic of material origin, age or process history. The ability to quantitatively identify new anthropogenic signatures from natural background signals is an important theme for forensic sciences. The characterization of vibrational structure of uranyl materials and minerals formed under environmental conditions will be used to evaluate spectra collected from anthropogenic uranium bearing materials and uranium minerals. Vibrational structure will be determined using Infrared and Raman Spectroscopies. Anthropogenic uranium – bearing materials will include uranium compounds commonly found throughout the mining and processing of uranium ore, fabrication of uranium fuel from uranium ore concentrates, and the reprocessing of spent uranium fuel, as well as, uranium bearing minerals. Here, we describe efforts in material synthesis and characterization of infrared absorption and Raman spectra and the instrumentation used to measure these signatures.

**Name:** Divya Banesh

**Program:** GRA

**School:** University of California, Davis

**Group:** CCS-7

**Mentor:** Ahrens, James Paul

**Category:** Computing

**Type:** Group Poster

**LA-UR:** 15-25435

# Advanced Exploration of Large-Scale Scientific Image Databases

Large-scale scientific simulations generate massive amounts of data, which can be a bottleneck for scientific discovery. “Cinema”, recently developed at Los Alamos National Laboratory and Kitware, Inc., achieves extreme scale in situ visualization by adopting an image-based approach for storing large-scale simulation data. Our application provides an interface to the Cinema database, allowing the scientist to view, cluster, query, and analyze images by leveraging the associated metadata. To get an overview of the complete space of images, the user is provided with a global view. The global view shows all images in a virtual 3D environment, where the alignment of images is defined by customizable context-dependent transformations of input dimensions such as time or viewpoint. A graphical interface allows the user to browse the Cinema database using metadata search as well as content-based image search. With metadata search, a scientist can look for images by querying the properties associated with the images. Additionally, with content-based search, given an image or part of image as input from the user, the program will return all images from the database that have similar features. The program will also provide existing trends or patterns that hold true over all images returned. Another way of grouping the images in the Cinema database based on physical variables such as temperature and pressure is the k-means clustering algorithm. This approach allows the scientist to recognize the underlying groups produced by the data set and the features associated with each group. The algorithm will be able to cluster the images on any number of physical variables represented by the database, as specified by the scientist. A web interface to the Cinema database completes the workflow by allowing the scientist to browse through the image database using the different techniques.

**Name:** David Barnes

**Program:** UGS/Postbacc

**School:** Massachusetts Institute of Technology

**Group:** CCS-7

**Mentor:** Lo, Li-Ta

**Category:** Computing

**Type:** Group Poster

**LA-UR:** 15-25435

# Advanced Exploration of Large Scale Scientific Image Databases

Large-scale scientific simulations generate massive amounts of data, which can be a bottleneck for scientific discovery. “Cinema”, recently developed at Los Alamos National Laboratory and Kitware, Inc., achieves extreme scale in situ visualization by adopting an image-based approach for storing large-scale simulation data. Our application provides an interface to the Cinema database, allowing the scientist to view, cluster, query, and analyze images by leveraging the associated metadata. To get an overview of the complete space of images, the user is provided with a global view. The global view shows all images in a virtual 3D environment, where the alignment of images is defined by customizable context-dependent transformations of input dimensions such as time or viewpoint. A graphical interface allows the user to browse the Cinema database using metadata search as well as content-based image search. With metadata search, a scientist can look for images by querying the properties associated with the images. Additionally, with content-based search, given an image or part of image as input from the user, the program will return all images from the database that have similar features. The program will also provide existing trends or patterns that hold true over all images returned. Another way of grouping the images in the Cinema database based on physical variables such as temperature and pressure is the k-means clustering algorithm. This approach allows the scientist to recognize the underlying groups produced by the data set and the features associated with each group. The algorithm will be able to cluster the images on any number of physical variables represented by the database, as specified by the scientist. A web interface to the Cinema database completes the workflow by allowing the scientist to browse through the image database using the different techniques.

**Name:** Gerald Collom

**Program:** UGS/Postbacc

**School:** University of Washington

**Group:** XCP-2

**Mentor:** Robey, Bob

**Category:** Computing

**Type:** Group Poster

**LA-UR:** LA-UR-15-25475

# Fast Mesh-to-Mesh Remaps Using Hash Algorithms

We explore the potential uses of hash-based algorithms in remapping values between computational meshes. We implement and test optimizations designed to reduce memory operations, and compare these optimizations in order to evaluate the performance impact across different meshes. Tests were run on 2-D meshes across various levels of mesh refinement and numbers of cells to measure the algorithms' relative speeds under differing circumstances.

**Name:** Jesse Giron

**Program:** UGS/Postbacc

**School:** Arizona State University

**Group:** XCP-3

**Mentor:** Trahan, Travis John

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25539

# MCATK Solid 3-D Geometries

The Monte Carlo Application ToolKit (MCATK) is a C++ software library designed to perform Monte Carlo transport of neutrons and photons. Recently, 3-D solid body geometry capabilities have been added to enable modeling of more complex geometries than can reasonably be modeled with the mesh-based geometries already implemented in MCATK. These geometries consists of shapes such as spheres, cylinders, boxes, and cones that can be translated and rotated in order to model a wide range of systems. The solid body geometry capability is being validated using the suite of criticality benchmarks also used by the Monte Carlo n-Particle Code (MCNP) and defined by the International Handbook of Evaluating Critical Safety Benchmark Experiments. These benchmarks range from a small sphere of radioactive material to models of nuclear reactors. The MCATK k-eigenvalue results are compared with the results obtained from MCNP. Preliminary tests and results show that the MCATK k-eigenvalue solutions obtained from the new 3-D solid body geometry are statistically agreeable with solutions obtained from MCNP. As of now, 24 of the 31 benchmark problems have been tested, while the remaining 7 will be completed in the near future.

**Name:** Jeremy Harrod

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** EES-16

**Mentor:** Makedonska, Nataliia

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25551

## Implementation of Feature Rejection Algorithm for Meshing using C++ Programming

DFNWorks is a software package developed at LANL, used in Discrete Fracture Network modeling. It simulates subsurface flow and transport in impermeable rocks such as granite, where fractures provide the main pathways for flow and solute transport. DFNWorks starts with fracture generation, then computational meshing, and lastly, flow and transport simulations. Fracture generation is currently done in Mathematica, and uses a Feature Rejection Algorithm for Meshing (FRAM). FRAM is a DFN generation technique, unique to DFNWorks and developed at LANL, which tests fractures for problematic features during DFN generation. Fractures, which cause problematic features, are rejected from the DFN on the fly. This ensures that the computational meshing phase will run smoothly and without problems. Mathematica was originally used for it's many built in functions, high precision, and ease of use. This allowed for faster validation of the FRAM algorithm. DFNWorks v1.0 is currently available for public use as free software, however, it still requires users to own Mathematica license. Also, very large DFNs can become difficult and time consuming due to the inability to control memory efficiently using Mathematica. The next version of DFNWorks is currently in development, which will resolve these issues. In the upcoming version, DFN generation will be done using C++. The need for Mathematica will be removed, making DFNWorks truly free software. DFNWorks will also be getting vastly improved memory management and run-time improvements for DFN generation. This latest version is soon to be in the testing and validation phase and will be released in the near future.

**Name:** Tamra Heberling

**Program:** GRA

**School:** Montana State University

**Group:** XTD-SS

**Mentor:** Terrones, Guillermo

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25394

## Simulation of a Hypervelocity Impact Experiment with PAGOSA Hydrocode

This work investigates how the Eulerian hydrocode PAGOSA performs while simulating a hypervelocity impact experiment of stainless steel 304-L into aluminum 6061-T6. The specifications of the simulation were established in a paper detailing an experiment conducted at the Atomic Weapons Establishment (AWE) in the UK and the Centre d'Etudes de Gramet (CEG) in France. A variety of strength models and equations of state were employed under several different mesh sizes. The results display an excellent comparison with the experimental data and demonstrate dramatic differences in impacted crater geometries over various strength models and mesh sizes.

**Name:** Andrew Hollis

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** A-2

**Mentor:** Tompkins, George

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25734

# Data Visualization for Threat Analytics

One of the most important things decision makers must take into account when they look at a problem are the threats that they face under various scenarios. When considering national security issues, for instance, policymakers must be aware of the threats that the nation faces from terrorists, diseases, weapons of mass destruction, hostile states, and many other factors. When analyzing these threats, decision makers often have to consider a multitude of variables. In order to make effective decisions, they not only have to be aware of what variables will impact threat levels, they also have to be aware of how these variables are related to one another. They have to know how different variables are interconnected and to what extent one variable effects another. Trying to analyze all these variables at once can be difficult. To make this analysis process more efficient, analysts often use data visualizations to communicate analysis insights in an intuitive way. This presentation will focus on the use of multidimensional R and JavaScript visualization tools to communicate threat levels under various scenarios. The presentation will explore how different visualizations can be used together to communicate threat levels, the connections between different variables, and the impact of particular variables on threat levels. The presentation will explain how decisions makers can use these visualizations to quickly understand what threats pose the greatest dangers, allowing them to use resources effectively to protect their assets.

**Name:** Jennifer Hu

**Program:** UGS/Postbacc

**School:** New Mexico State University

**Group:** CCS-7

**Mentor:** Baker, Zachary Kent

**Category:** Computing

**Type:** Group Poster

**LA-UR:** LA-UR-15-25473

# Detecting and Curve Fitting EMPs in the Ionosphere

This project's purpose is analyze a wide-band radio-frequency (RF) events detected via space-based radio receivers onboard GPS spacecraft. This software receives data from a pre-filter that captures wide-band events, but does not attempt to discriminate between interesting events, such as lightning and EMP, and uninteresting events, such as on-board discharges (OBD, sparking between electrically isolated parts of the spacecraft). RF energy that has passed through the ionosphere has a characteristic dispersion shape; this is indicated by a inverse quadratic delay as a function of the frequency and total electron content (TEC) of the path through the ionosphere; RF energy that has not passed through the ionosphere tends to have no frequency dependent delay. The goal of our research is to distinguish between trans-ionospheric events and false events (such as static discharge, noise, etc.), and then forward interesting events for further analysis. The system channelizes wideband ADC records using fixed-point sub-band tuner code in C. The sub-band tuner is based on a fixed-point FIR implementation, and the down-sampling is done via simple decimation technique. A curve fitting routine, using the least squares fitting method will be applied to the data at multiple frequency domains to estimate the amount of TEC in a captured event. We attempt to improve the curve fit by iteratively improved to remove outliers and weighting data points based on SNR. A decision to keep data would then be based on the output of the TEC estimation.

**Name:** David Hyde

**Program:** GRA

**School:** Stanford University

**Group:** XCP-4

**Mentor:** Schmidt, Joseph H

**Category:** Computing

**Type:** Group Poster

**LA-UR:** LA-UR-15-25476

# Survey of Multi-Material Closure Models in 1D Lagrangian Hydrodynamics

Accurately treating the coupled sub-cell thermodynamics of computational cells containing multiple materials is an inevitable problem in hydrodynamics simulations, whether due to initial configurations or evolutions of the materials and computational mesh. When solving the hydrodynamics equations within a multi-material cell, we make the assumption of a single velocity field for the entire computational domain, which necessitates the addition of a closure model to attempt to resolve the behavior of the multi-material cells' constituents. In conjunction with a 1D Lagrangian hydrodynamics code, we present a variety of both the popular as well as more recently proposed multi-material closure models and survey their performances across a spectrum of examples. We consider standard verification tests as well as practical examples using combinations of fluid, solid, and composite constituents within multi-material mixtures. Our survey provides insights into the advantages and disadvantages of various multi-material closure models in different problem configurations.

**Name:** Marina Kiseleva

**Program:** UGS/Postbacc

**School:** Virginia Polytechnic Institute and State University

**Group:** HPC-5

**Mentor:** Ionkov, Latchesar Alexandrov

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** 15-25704

# Input/Output Optimizations Using Low Level Virtual Machine (LLVM)

The purpose of this project is to increase Input/Output performance by using bitcode to manipulate the I/O calls of a program. Using the open-source software LLVM (the Low Level Virtual Machine project from the University of Illinois) with the front end Clang, we will write a "pass" to traverse over the bitcode of a program to optimize it internally. This traversal will detect all I/O calls and translate them into asynchronous I/O that can occur in the background, therefore reducing the I/O latency. Our solution furthermore prevents dirty reads and writes by maintaining all the current I/O processes and ensuring they do not interfere with one another. This project will improve overall execution time and I/O performance for virtually any program, as LLVM is a language-anonymous software.

**Name:** Sebastian Klaassen

**Program:** GRA

**School:** University of Vienna

**Group:** CCS-7

**Mentor:** Ahrens, James Paul

**Category:** Computing

**Type:** Group Poster

**LA-UR:** 15-25435

# Advanced Exploration of Large-Scale Scientific Image Databases

Large-scale scientific simulations generate massive amounts of data, which can be a bottleneck for scientific discovery. “Cinema”, recently developed at Los Alamos National Laboratory and Kitware, Inc., achieves extreme scale in situ visualization by adopting an image-based approach for storing large-scale simulation data. Our application provides an interface to the Cinema database, allowing the scientist to view, cluster, query, and analyze images by leveraging the associated metadata. To get an overview of the complete space of images, the user is provided with a global view. The global view shows all images in a virtual 3D environment, where the alignment of images is defined by customizable context-dependent transformations of input dimensions such as time or viewpoint. A graphical interface allows the user to browse the Cinema database using metadata search as well as content-based image search. With metadata search, a scientist can look for images by querying the properties associated with the images. Additionally, with content-based search, given an image or part of image as input from the user, the program will return all images from the database that have similar features. The program will also provide existing trends or patterns that hold true over all images returned. Another way of grouping the images in the Cinema database based on physical variables such as temperature and pressure is the k-means clustering algorithm. This approach allows the scientist to recognize the underlying groups produced by the data set and the features associated with each group. The algorithm will be able to cluster the images on any number of physical variables represented by the database, as specified by the scientist. A web interface to the Cinema database completes the workflow by allowing the scientist to browse through the image database using the different techniques.

**Name:** Nicholas Lewis

**Program:** GRA

**School:** University of Minnesota, Twin Cities

**Group:** HPC-3

**Mentor:** Connor, Carolyn Marie

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-24801

## Nuclear Testing, Weapons Strategy, and Supercomputer Selection at Los Alamos

Since its beginnings during the Manhattan Project, the Laboratory at Los Alamos has employed advanced scientific computing in the performance of its evolving mission. Beginning with human computers equipped with desk calculators, and later employing electromechanical, then high-speed digital computing equipment, the forms and capabilities of the computers at Los Alamos directly impacted its ability to meet and fulfill its responsibilities as a scientific and national laboratory. As a consequence, the supercomputer selection process employed at the Lab provides valuable insights into the pressures, drives, and influences that shaped Lab computing, highlighting how those who selected the Lab's most powerful computers perceived and imagined the role and future directions of Los Alamos during the Cold War. In the mid-1960s, when Los Alamos embarked on a search for a new supercomputer to ease the burden on its saturated computer facilities, the selection committee envisioned vastly different computing demands than would exist at the Lab in only a few years' time. The committee, based on its assumptions and experiences with supercomputing up to 1964, initially predicted a gradual increase in computing demand, when, by contrast, the late 1960s marked the beginning of a wholesale expansion in computer power and use at Los Alamos. Why did the selection committee, comprised of some of the foremost experts of their time on supercomputing in the lab system, anticipate a markedly different computing demand and environment than emerged in only a few years' time? This poster argues that changes in nuclear testing policy, the maturation of weapons design, and changes in weapons strategy, greatly altered the demands upon computing at Los Alamos, spurring a rapid escalation in computing capacity that even Lab computing insiders could not have anticipated.

**Name:** Jungyeoul Maeng

**Program:** GRA

**School:** The University of Michigan

**Group:** XCP-4

**Mentor:** Schmidt, Joseph H

**Category:** Computing

**Type:** Group Poster

**LA-UR:** LA-UR-15-25476

## Survey of Multi-Material Closure Models in 1D Lagrangian Hydrodynamics

Accurately treating the coupled sub-cell thermodynamics of computational cells containing multiple materials is an inevitable problem in hydrodynamics simulations, whether due to initial configurations or evolutions of the materials and computational mesh. When solving the hydrodynamics equations within a multi-material cell, we make the assumption of a single velocity field for the entire computational domain, which necessitates the addition of a closure model to attempt to resolve the behavior of the multi-material cells' constituents. In conjunction with a 1D Lagrangian hydrodynamics code, we present a variety of both the popular as well as more recently proposed multi-material closure models and survey their performances across a spectrum of examples. We consider standard verification tests as well as practical examples using combinations of fluid, solid, and composite constituents within multi-material mixtures. Our survey provides insights into the advantages and disadvantages of various multi-material closure models in different problem configurations.

**Name:** Christopher Moore

**Program:** UGS/Postbacc

**School:** University of Kentucky

**Group:** HPC-3

**Mentor:** Mason, Michael A

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25512

# Monitoring High Performance Computing Systems for the End User

Monitoring of High Performance Computing clusters is currently geared towards providing system administrators the information they need to make informed decisions on the resources used in the cluster. However, this emphasis leaves out the End User, those who utilize the cluster resources towards projects and programs, as they are not given the information of how their workflow is impacting the cluster. By providing a subset of monitoring data in a format End Users can easily interpret and utilize, they can help make better use of the computing resources provided to them.

**Name:** Heidi Morning

**Program:** GRA

**School:** University of California at Davis

**Group:** HPC-3

**Mentor:** Cunningham, Rob

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25312

# Characterizing and Optimizing Lustre I/O Performance on LANL HPC Systems

There is considerable emphasis for scientific applications to efficiently use the processors in high-performance computing systems. However, I/O operations, such as reading or writing to the file system, can significantly affect runtimes and be the primary performance bottleneck. Currently, HPC Division platforms employ two parallel file system architectures, Panasas and Lustre, whose primary purpose is to provide temporary high-speed I/O between HPC clusters and online disk storage. Panasas is HPC's legacy file system and will soon be replaced by the more efficient Lustre file system. This project examines Lustre's I/O performance on LANL HPC clusters to provide a comprehensive performance characterization and to guide LANL users on potential I/O optimizations. To characterize Lustre's efficiency, the following tests were performed: I/O caching due to file size, the effects of transfer size on I/O, I/O ramifications due to scaling, and the differences of I/O performance when using various APIs— POSIX, MPIIO, and HDF5. Furthermore, the previously stated tests were performed using two different configuration models: file-per-process and single shared file. These results will be provided to users to give them realistic expectations for I/O performance for their respective applications and provide useful I/O optimization strategies when using the Lustre file system.

**Name:** Miguel Pacheco

**Program:** UGS/Postbacc

**School:** Northern New Mexico College

**Group:** DCS-CSD

**Mentor:** Esquibel, Le'Andrea

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25622

# ESD: Automating Monthly Financial Reports

Presentation Abstract: The DCS-CSD Electronic Software Distribution (ESD) enterprise service, enables LANL employees to purchase, install, and manage software licenses. ESD is responsible for the tracking, managing, and billing of all the licenses. Our job is to automate the monthly financial reports and have a seamless interaction with the monthly billing/payment process. We use the asp.NET framework to create web applications to make an easy to use graphical user interface (GUI). The GUI allows the ESD Financial Administrator to input information such as a range of dates that specifies what information should be returned. Behind the web application we use SQL Server Agent jobs on a Microsoft SQL server database. The SQL agent jobs use database stored procedures to query the database. The new processes have reduced the time and effort needed by the ESD financial team to create reports needed each month. Most of the monthly reports have been automated with the exception of one or two that are currently in the process of being converted

**Name:** Zhuolin Qu

**Program:** GRA

**School:** Tulane University

**Group:** EES-16

**Mentor:** Makedonska, Nataliia

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25550

# Efficient & Parallelized Computing of Control Volumes for HPC Flow Solvers

Interconnected networks of fractures act as the principal pathways for transport in relatively impermeable rocks. The discrete fracture network (DFN) model explicitly represents these fractures and therein resolves flow and transport of solutes through the subsurface. Over the past 5 years, the Subsurface Flow and Transport team (EES-16) at the Los Alamos National Laboratory has developed dfnWorks, a HPC computational suite for modeling flow and transport in large DFNs. The first step to resolving flow and transport in a DFN is the generation of a high-quality mesh from which control volumes for HPC finite volume solvers can be obtained. In dfnWorks a conforming Delaunay mesh is produced, and then the dual Voronoi mesh is passed to the finite volume solver. However, computing the volume and areas associated with the Voronoi diagram can be computationally expensive, especially for large DFNs with hundreds of millions of control volumes. To reduce the memory overhead and CPU time, we developed and implemented a new methodology that is based on dynamic data structures and operates in parallel using PETSc (Portable, Extensible Toolkit for Scientific Computation) toolkit and MPI (Message Passing Interface). Comparisons with the previous computation of the Voronoi diagrams show significant reduction of memory usage and wall clock times.

**Name:** Andres Quan

**Program:** UGS/Postbacc

**School:** New Mexico Institute of Mining and Technology

**Group:** CCS-7

**Mentor:** Braithwaite, Ryan

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25520

# Smart Node Allocation and Statistics Gathering

Heterogeneous clusters such as Darwin, held here at Los Alamos National Laboratory, contain unique groups of computers that allow researchers in Computer Science, to test their code on a variety of different hardware. Darwin consists of partitions that range from ones with monstrous amounts of RAM, to partitions with as many as 72 cores per node. This differs from typical supercomputers where all the nodes are identical. The issue with a system such as Darwin is that it is typically difficult to allocate the exact resources that one would need for a project. Unless one is the system administrator, or one is willing to memorize the names of the nodes that are needed, having good control over the system and knowing what is there, is a laborious task. Utilities such as SLURM (Simple Linux Utility for Resource Management) provide some amount of control, however it does not provide information about hardware. The solution to such a problem is a tool I have created known as Slurm Command. This is a system that consists of scripts that execute on the login node to dump raw system information from the Linux “proc” directory of each node to be processed and sent to a MySQL server for daily statistics about the hardware on Darwin. The data is then downloaded by a client, which provides the user with a method to automatically allocate the fastest available node that contains the hardware needed by that user.

**Name:** Colin Redman

**Program:** UGS/Postbacc

**School:** Arizona State University

**Group:** XCP-2

**Mentor:** Robey, Bob

**Category:** Computing

**Type:** Group Poster

**LA-UR:** LA-UR-15-25475

# Fast Mesh-to-Mesh Remaps using Hash Algorithms

We explore the potential uses of hash-based algorithms in remapping values between computational meshes. We implement and test optimizations designed to reduce memory operations, and compare these optimizations in order to evaluate the performance impact across different meshes. Tests were run on 2-D meshes across various levels of mesh refinement and numbers of cells to measure the algorithms' relative speeds under differing circumstances.

**Name:** Miri Ryu

**Program:** GRA

**School:** University of New Mexico

**Group:** HPC-5

**Mentor:** Chen, Hsing Bung

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25454

# Erasure Coding In SIMD Platform Is More Cost-Efficient Than In x86 Platform

Erasure coding based storage system is one of the most powerful alternative to replace the traditional multiple data replication model of HPC and cloud storage systems because it is more cost-efficient as well as it is able to endure as much data failure as customized. SIMD(Single Instruction, Multiple Data) is data level parallelism that applies single instruction onto an array of data concurrently. Both erasure encoding and decoding processes involve computation of intensive mathematic operations such as addition (XOR), multiplication on array, matrix, and logarithm and an antilogarithm table-lookup. Given the compute-intensive nature of erasure code computing, it is worth considering whether utilizing vector instructions from SIMD extensions is suitable for large scale erasure code based cloud storage systems. In this project, we launch single encoding process and multiple concurrent encoding processes on a multicore computer system and we conduct studies of encoding performance, power consumption, and energy efficiency of erasure code computing. We evaluate erasure code computing process using both Intel x86 platform and Intel Streaming SIMD extension platform. We apply a breakdown analysis approach on power consumption measurement of erasure code encoding. We present the impact of vectorization on erasure coding procedure in terms of reducing processing time, reducing power utilization, and energy cost. Finally we conclude our studies and demonstrate the Intel x86's Streaming SIMD extensions computing is a cost-effective and favorable choice for future power efficient HPC cloud storage systems.

**Name:** Emma Schmidt

**Program:** UGS/Postbacc

**School:** New Mexico Institute of Mining and Technology

**Group:** XTD-NTA

**Mentor:** Green, Andrew Allan

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25352

# Utilizing the Gruneisen Equation of State in the Noh Shock Test Problem

The Gruneisen equation of state is a relevant model for many materials, in part because it has a variety of mathematical representations. Incorporating a wide array of these forms into multiphysics codes expands the field of problems we can simulate. Our primary focus has been to investigate the implementation and relevance of various forms of the Gruneisen equation of state in the Lagrangian hydrocode FLAG. The FLAG hydrocode's existing Gruneisen forms include six to eleven user settable parameters. These parameters and their specifications are not always applicable; expanding the available forms allows greater flexibility. In anticipation of new analytic solutions that utilize the Gruneisen equation of state, our Gruneisen form is customized to provide the necessary infrastructure. In order to preserve compatibility with the existing code infrastructure and user base, our modifications only include variants of the existing Gruneisen forms. This method opens the possibility for future users to tailor a Gruneisen equation of state to their specific simulations. The Noh code-verification problem allows us to test our modifications against an exact solution, and allows us to see how this form behaves in a simulation with an analytic solution.

**Name:** Uzma Shaikh

**Program:** GRA

**School:** Purdue University, West Lafayette, In

**Group:** CCS-7

**Mentor:** Rogers, David Honegger

**Category:** Computing

**Type:** Group Poster

**LA-UR:** LA-UR-15-25435

# Advanced Exploration of Large-Scale Scientific Image Databases

Large-scale scientific simulations generate massive amounts of data, which can be a bottleneck for scientific discovery. "Cinema", recently developed at Los Alamos National Laboratory and Kitware, Inc., achieves extreme scale in situ visualization by adopting an image-based approach for storing large-scale simulation data. Our application provides an interface to the Cinema database, allowing the scientist to view, cluster, query, and analyze images by leveraging the associated metadata. To get an overview of the complete space of images, the user is provided with a global view. The global view shows all images in a virtual 3D environment, where the alignment of images is defined by customizable context-dependent transformations of input dimensions such as time or viewpoint. A graphical interface allows the user to browse the Cinema database using metadata search as well as content-based image search. With metadata search, a scientist can look for images by querying the properties associated with the images. Additionally, with content-based search, given an image or part of image as input from the user, the program will return all images from the database that have similar features. The program will also provide existing trends or patterns that hold true over all images returned. Another way of grouping the images in the Cinema database based on physical variables such as temperature and pressure is the k-means clustering algorithm. This approach allows the scientist to recognize the underlying groups produced by the data set and the features associated with each group. The algorithm will be able to cluster the images on any number of physical variables represented by the database, as specified by the scientist. A web interface to the Cinema database completes the workflow by allowing the scientist to browse through the image database using the different techniques.

**Name:** Ryan Slechta

**Program:** UGS/Postbacc

**School:** University of St. Thomas

**Group:** HPC-5

**Mentor:** Debardeleben, Nathan

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25673

# Resilience Testing of a Top K Selection Algorithm

Factors such as cosmic rays, radioactive packaging, and thermal neutrons are known to be the primary source of soft errors in that they may cause data to be corrupted at a program's runtime. In this paper, we investigate the effects of both probability and pivot choice on the resilience of a particular selection algorithm to soft errors. To do this, we employ a Fine-grained Soft Error Fault Injection tool (FSEFI) that allows the injection of fault at arbitrary rates. Finally, we assess various applications of the selection algorithm, and we investigate different metrics of error, optimizing for the application in mind.

**Name:** Hunter Stuckey

**Program:** GRA

**School:** New Mexico State Univerity

**Group:** CCS-7

**Mentor:** Baker, Zachary Kent

**Category:** Computing

**Type:** Group Poster

**LA-UR:** 15-25473

## Detecting and Curve Fitting EMPs in the Ionosphere

This project's purpose is to analyze wide-band radio-frequency (RF) events detected via space-based radio receivers on-board GPS spacecraft. This software receives data from a pre-filter that captures wide-band events, but does not attempt to discriminate between interesting events, such as lightning and EMP, and uninteresting events, such as on-board discharges (OBD, sparking between electrically isolated parts of the spacecraft). RF energy that has passed through the ionosphere has a characteristic dispersion shape; this is indicated by a inverse quadratic delay as a function of the frequency and total electron content (TEC) of the path through the ionosphere; RF energy that has not passed through the ionosphere tends to have no frequency dependent delay. The goal of our research is to distinguish between trans-ionospheric events and false events (such as static discharge, noise, etc.), and then forward interesting events for further analysis. The system channelizes wide-band ADC records using fixed-point sub-band tuner code in C. The sub-band tuner is based on a fixed-point FIR implementation, and the down-sampling is done via simple decimation technique. A curve fitting routine, using the least squares fitting method will be applied to the data at multiple frequency domains to estimate the amount of TEC in a captured event. We attempt to improve the curve fit by iteratively improved to remove outliers and weighting data points based on SNR. A decision to keep data would then be based on the output of the TEC estimation.

**Name:** Nicholas Torres

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** CCS-7

**Mentor:** Tripp, Justin Leonard

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25436

# Optimizing Data Movement to and from a SpaceWire Endpoint

The Joint Architecture Standard (JAS) is a joint project between Los Alamos National Laboratory and Sandia National Laboratories to provide a common processing and communication infrastructure upon which to more quickly develop payload sensing and processing capabilities. JAS offers a flexible, scalable, and reliable solution to space-based processing for our customer's applications. SpaceWire is used by JAS for payload command and control as well as low rate mission data routing. SpaceWire provides standard computing and data services for a wide range of sensor systems that may consist of a small simple network of only a few nodes, to a large complex network of hundreds of nodes. The purpose of this work is to improve the efficiency of the bridge between the microprocessor and the space wire physical layer interface (phy). When sending data the microprocessor would originally poll a register in the SpaceWire phy and then write 9 bits to a FIFO, which is used to store data that it receives or hold data it is going to send. Polling a register from the software takes a few clock cycles which limits the speed at which data is able to be sent or read from a FIFO. When SpaceWire starts running at faster speeds a higher percentage of relative time is wasted polling registers and slowly writing a small amount of data into a FIFO. Our new approach uses DMA(Direct memory access), and is able to write 32 bits of data from one memory address to another memory address every clock cycle. In addition to the DMA, interrupts are also used which allows the CPU to avoid polling. This allows the CPU to complete other tasks while waiting for an interrupt. The DMA and interrupts allowed data to reach the SpaceWire FIFO quicker.

**Name:** Steven Wong

**Program:** GRA

**School:** Norfolk State University

**Group:** NEN-3

**Mentor:** Dickens, Brian Scott

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25657

# Collecting Data from a Wind Station

A LANL team is predicting the paths of pathogens released in the air from terrorist attacks or industrial accidents in major American cities. They need wind data as input to make these predictions, and we are addressing that need. The purpose of my work was to create a networked computer service to provide wind data on demand for a dynamic runtime geo-domain. I used Windows Communication Foundation, C#, and Visual Studio 2013 to create the service. My Service collects wind data from weather monitoring stations directly provided by MesoWest, http://mesowest.utah.edu/. One challenge is this project is quickly inserting large amounts of data into a SQL database. We will examine several algorithms for improving SQL insert efficiency.

**Name:** Johnnie Wright

**Program:** UGS/Postbacc

**School:** Santa Fe Community College

**Group:** A-1

**Mentor:** Del Valle, Sara Yermimah

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** 15-25683

## Anti-Vaccine Twitter Hashtags are Predictive of Vaccine Preventable Disease

We explored the correlation between anti-vaccine related hashtags and preventable disease incidence in California. According to the Centers for Disease Control and Prevention (CDC), vaccines have saved over half a billion lives since the middle of the 20th century, yet a growing anti-vaccination sentiment threatens to compromise the future of their efficacy. Understanding this negative sentiment has proved difficult in the past due to our inability to measure how these communities form and examine their impact on the general public. In order to analyze this phenomenon, we propose using the free social networking service, Twitter, to measure the prevalence of these hashtags. Previous efforts on the effects of Twitter have proven the platform's ability to track human behavior through keywords with success. We gathered 1 percent of all twitter data from January 2010 to April 2015 in order to analyze the hashtags related to anti-vaccination, and measured their frequency in relation to preventable disease outbreaks. Our preliminary results show that the Twitter posts related to an emerging anti-vaccination movement produce a positive correlation for pertussis,and seasonal influenza. Measles appears to be unaffected by this data. Based on these results, we conclude that social media continues to be an effective way of examining the spread of sentiment between communities online and terrestrial. It may be useful on educating these communities apprehensive about vaccinations in order to reduce outbreak incidence.

**Name:** Christopher Wu

**Program:** GRA

**School:** University Of New Mexico

**Group:** HPC-5

**Mentor:** Chen, Hsing Bung

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** 15-25452

## Power Consumption and Performance Studies of Erasure Code Computing

The cost to maintain the storage of petabytes of data with recovery costs millions each year that can be reduced by increasing the efficiency of encoding/decoding data with parity, and choosing a cost efficient storage device. This project uses a Shingled Magnetic Recording (SMR) hard drive and a Flash memory hard drive to compare their processing time, encoding bandwidth, and cost per gigabyte. Multiple data replication redundancy is a costly process that requires up to twice or thrice the amount of hard drives to copy the data bit by bit. This method requires more hardware and maintenance compared to erasure code storage. For this experiment, the setup is as follows: a work machine, a watts up? power meter and the Watts Up Real Time program, and a Fedora 21 test machine. The power meter measures the watts used by the test machine every second while the machine encodes a 40GB file with erasure code. The results from the power meter are recorded on the work machine in Watts Up Real Time. Watts, encoding speed, and processing time are recorded to a spreadsheet. In the project, we conducted performance studies of Power consumption and performance studies of erasure code computing on Flash based and SMR (Shingled Magnetic Recording) based storage devices.

**Name:** Qing Zheng

**Program:** GRA

**School:** Carnegie Mellon University

**Group:** HPC-5

**Mentor:** Settlemyer, Bradley Wade

**Category:** Computing

**Type:** Individual Poster

**LA-UR:** 15-25301

# BatchFS: Ultrascale File System Metadata Funded by Client Applications

Parallel file systems are often characterized by a layered architecture that separates metadata from data operations. Yet metadata intensive workloads can still bottleneck at the file system metadata path due to namespace synchronization typically offered by a single or a few dedicated metadata servers. To better accommodate batch workloads common in HPC environments, we propose a client-driven file system metadata architecture named BatchFS. To avoid metadata bottlenecks, BatchFS features a relaxed consistency model and optimistic concurrency control. Capable of executing namespace operations on client-provisioned resources without contacting any dedicated servers, BatchFS clients are able to delay namespace synchronization until that is really needed. Experiments demonstrate that BatchFS outperforms a traditional parallel file system by orders of magnitude.

**Name:** Daniel Ahrens

**Program:** UGS/Postbacc

**School:** University of California- Berkeley

**Group:** EES-14

**Mentor:** Rowland, Joel C

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25484

## Permafrost Controls on Sediment Transport in Arctic Rivers: A Study on the Yukon

As temperatures rise due to climate change, Arctic ecosystems become more susceptible to change, particularly ones dominated by the presence of permafrost. Quantifying the role of permafrost soils on riverbanks is important to understanding sediment transport in Arctic rivers. Permafrost is hypothesized to be a control on erosion rates because frozen soils are thought to protect riverbanks from erosion and limit sediment input from the banks into the river. However, no such effect has been definitively quantified in the field. We hope to investigate the possibility of this effect utilizing remote-sensing techniques. Studying these sediment cycles in Arctic regions is critical to understanding the impact of climate change on Arctic aquatic ecosystems. The project attempts to understand the impact of permafrost on erosion rates on the Yukon River using Landsat satellite imagery and USGS permafrost probability maps. The Yukon River was selected due to the availability of permafrost and satellite data. This project studies the effect of permafrost on the rates of river channel bank erosion. We hope to understand reach behavior by developing a tool to measure permafrost's impact. Utilizing output from the Spatially Continuous Riverbank Erosion and Accretion Measurements (SCREAM) software package, a river analysis program developed at LANL, we wrote software that traces historic erosion rates as a function of current permafrost levels. By comparing historic erosion rates to current permafrost extent, this project will test if permafrost has any measurable impacts on erosion rates. The results from this study will help build a more comprehensive model of sediment transport in the Arctic.

**Name:** Sara Beroff

**Program:** UGS/Postbacc

**School:** UC- Berkeley

**Group:** EES-14

**Mentor:** Ding, Mei

**Category:** Earth & Space Sciences

**Type:** Group Poster

**LA-UR:** 15-25485

# Sediment Particle Size Distribution from Core Holes of the LANL Chromium Plume

Between 1956 and 1972, between 31,000 and 72,000 kg of chromium used in laboratory cooling towers was released as effluent into Sandia Canyon. As a result, the aquifer underneath laboratory property is contaminated with high levels of chromium (VI), a toxin and carcinogen. Sampling groundwater monitoring wells on laboratory property provides information on the behavior of the chromium plume. For groundwater to enter a monitoring well, it must pass through a screen at the bottom. An optimal screen for these monitoring wells will allow groundwater to pass through while keeping out sediments. A particle size analysis of aquifer materials categorizes the subsurface material into sand, silt, or gravel. This information will help engineer better well screens and provide a better understanding of how water flows through the aquifer. Samples from five different core holes within the chromium plume were collected via sonic drilling at depths ranging from 732'-1125'. To obtain a particle size analysis, the samples were sieved into six different particle size fractions, of >4 mm, 2-4 mm, 1.4-2 mm, 0.355-1.4 nm, 180-355 µm, and smaller than 180 µm. The mass distributions were then plotted against their corresponding sieve size. The sample material was mostly from the Puye formation, a poorly sorted formation containing sedimentary rocks that have been pushed down from the Jemez volcanic field. The remaining samples were Miocene pumiceous, a poorly sorted pumice. The particle sizes were mostly silt, with some sands and gravels. The data demonstrated that there was a variety in sample material and size in the subsurface. The results of this study provide site-specific information in support of long-term monitoring well operations for chromium plume investigation and remediation.

**Name:** Jeremy Brunette

**Program:** GRA

**School:** The University of Nevada,Reno

**Group:** ENV-ES

**Mentor:** Purtzer, LeAnn Carol

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25479

## S-Site Stories: Utilizing Compliance Data to Understand the Manhattan Project

In 1942, the construction of the world's first atomic weapon was approved by President Franklin Delano Roosevelt. Brigadier General Leslie Groves was appointed to take complete executive charge of the program. Groves chose J. Robert Oppenheimer to serve as the scientific director for The Manhattan Project, also known as Project Y. The top secret nature of Project Y required an isolated location for the design and construction of the atom bomb, and Los Alamos, New Mexico was determined to be a suitable location. To support of the development of the first atomic weapons, including the "Trinity" bomb, and those dropped on Hiroshima (Little Boy) and Nagasaki (Fat Man) the S-Site (TA-16) was constructed as a high explosives laboratory at Los Alamos. The hazardous nature of high explosives necessitated the location of S-Site well away from the Los Alamos town site. Many of the Manhattan Project period buildings have been decommissioned and demolished. In accordance with the National Historic Preservation Act (NHPA), and Executive Order 1153, twenty-seven of the buildings, and one structure were surveyed, photographed and documented prior to demolition. Because these buildings have been decommissioned, the completed survey holds great importance, as it provides an accurate architectural documentation of the building as they were originally built and how they were in their final condition. The survey documentation also documents the activities associated with each building. Current efforts to organize and distribute the information found in this survey is germane to the creation of the Manhattan Project National Historic Park, and provide an opportunity to further understand the events related to the creation of the Atomic bomb.

**Name:** Amanda Cvinar

**Program:** GRA

**School:** Adams State University

**Group:** ENV-ES

**Mentor:** Purtzer, LeAnn Carol

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25477

# Nominating a National Historic Landmark on the Pajarito Plateau

The Mortandad Cavate Complex and associated Sandia Pueblo are two archaeological sites located within Los Alamos National Laboratory (LANL) that exhibit an exceptional level of preservation and integrity. These sites, designated by the Laboratory of Anthropology number LA 12609, are one of four Ancestral Pueblo sites that the Department of Energy (DOE) plans to nominate as a National Historic Landmark (NHL). The remains of the Mortandad Cavate Complex and Sandia Pueblo are included in the traditions of the Pueblo de San Ildefonso and may represent a place of special cultural and traditional value. LA 12609 includes 163 cavate rooms including the cave kiva, prehistoric trails, and an associated mesa top pueblo, Sandia Pueblo. The site dates to the Ancestral Pueblo Late Coalition and Early Classic periods (A.D. 1225-1350) and the distribution of archaeological features follows the east to west orientation along the south facing cliff face of Mortandad Canyon. National Historic Landmarks are historic places that possess exceptional value in commemorating or illustrating the history of the United States. There are approximately 2,500 National Historic Landmarks and the designation of a property as a NHL ensures that stories of nationally important historic events, places, or persons are recognized and preserved for the benefit of all citizens. The purpose of this project is to plan and execute fieldwork needed in order to complete and submit the NHL nomination of LA 12609. Extensive recording and documentation of the sites will be conducted and an in-depth context drafted for the history of these sites on the Pajarito Plateau during the late prehistoric period. This project will require a collaborative effort between the Pueblo de San Ildefonso, the LANL visual team, and the Environmental Stewardship Services Cultural Resources Team to produce the documentation of this NHL on the Parjarito Plateau.

**Name:** Sean Dolan

**Program:** GRA

**School:** University of Oklahoma

**Group:** ENV-ES

**Mentor:** Purtzer, LeAnn Carol

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25470

## Prehispanic Patterns of Obsidian Procurement on the Pajarito Plateau

The transition between the Coalition and Classic periods in the late thirteenth and early fourteenth centuries A.D. was a time of immense demographic transformation, social reorganization, and coalescence, as thousands of people left the Mesa Verde region in southwestern Colorado and migrated south into the Pajarito Plateau. This inevitably shaped the historical and cultural trajectory for future generations of Ancestral Pueblo people along the northern Rio Grande. Multiple lines of evidence have been used to examine how, when, and why people left, but archaeological research has generally focused on the donating Mesa Verde side, and not on how people in the Pajarito Plateau were affected as a result of the influx of diasporic communities entering. Using data generated by X-ray fluorescence analysis on obsidian stone tools collected during Los Alamos National Laboratory's Land Conveyance and Transfer Data Recovery Project, and from Bandelier National Monument, I examine if the in-migration process affected obsidian source-use prior to, during, and after, the Coalition to Classic transition, like it did to other aspects of life. I present my findings using multiscalar analyses (macro, meso, micro) because each scale yields a different understanding of obsidian procurement through time and across space. This approach allows for a more dynamic account of which obsidian sources people used during one of the most important events in the prehispanic North American Southwest. Macroscale analyses demonstrate people predominantly used Cerro Toledo obsidian from the Jemez Mountains. Looking diachronically and spatially using the mesoscale and microscale, however, there are differences between the use of Cerro Toledo and Cerro del Medio during the Coalition and Classic periods, and at archaeological sites in the north at LANL and in the south at Bandelier. These differences are likely a result of changing practices and traditions of obsidian procurement because of transformations in demography.

**Name:** Jordan Fonseca

**Program:** UGS/Postbacc

**School:** University of Puget Sound

**Group:** ISR-1

**Mentor:** Walker, Andrew Charles

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25499

## Validation Study of the C++ Cloud Lofting Module for DIORAMA

A cloud lofting module that models the vertical location of nuclear clouds is tuned to best match observed cloud heights through an error minimization study. The cloud lofting module serves to modify the location of delayed gamma ray emission from the cloud and hence, the atmospheric signal attenuation after a nuclear detonation. The cloud lofting module is a part of the DIORAMA infrastructure - a validation program for the entire space-based nuclear detonation detection system. No validation study of the C++ nuclear cloud lofting code for the DIORAMA project exists, and older models such as Jodoin (1994), Norment (1979), and Huebsch (1964) contain known errors. Additionally, previous models explored only a small range of values for two of the empirical parameters. Furthermore, the empirical entrainment parameter is known to compensate for a known cloud surface area error. This validation study expands the parameter space to minimize the error in the observed cloud top and bottom heights. Ranges for three empirical parameters measuring entrainment, μ, kinetic to turbulent energy conversion, k2, and turbulent energy dissipation rate, k3, are selected using an iterative brute-force method. The fractional root-mean-square (RMS) error is computed across 54 nuclear detonation tests from observational data (Hawthorne, 1979). Regions in the parameter space near local minima are explored more thoroughly in an iterative process, and RMS error is successively reduced. Average FRMS error is minimized at 0.22 for $\mu = 0.1$, $k2 = 5.0$, and $k3 = 5.0$ corresponding to a top cloud height FRMS error of 0.18 and a bottom cloud height FRMS error of 0.30. Possible correlations between FRMS error and the cloud height of burst and device yield are also explored.

**Name:** Patrick Gasda

**Program:** UGS/Postbacc

**School:** New Mexico Tech

**Group:** ISR-2

**Mentor:** Wiens, Roger Craig

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25456

# Compositions of Feldspars from Mars

Compositions of Feldspars from Mars  The NASA Curiosity rover studies the Martian surface using ChemCam, a laser-based elemental analysis instrument. A focused laser ionizes a small point on a rock, and the ionized elements emit light at characteristic wavelengths that are recorded by a spectrometer. The ChemCam team has developed a new calibration technique that has greater major-element analysis accuracy. Using this technique, we have found 125 likely feldspar (alkali alumino-silicate minerals indicative of magma composition and stage of chemical evolution) targets that were measured during the first 801 Martian days of the rover mission. Sixty one percent of the feldspars analyzed have approximately equal proportions of Na and Ca, implying the parent magmas likely formed directly from the mantle. Thirty four of the targets were Na-dominant, indicating magmas evolved from the direct mantle source. Only six targets are Ca-dominant, indicating that most magmas form at a relatively lower temperature. Eight targets contain high of potassium. The amount of potassium is proportional to the degree of evolution of the magma in a magma chamber. These results suggest that Mars forms magma chambers from melting in the mantle, and these mantle chambers erupt and chemically evolve over time. Magmatic differentiation can only take place in reasonably thick crust, so one would expect to find Na-rich feldspars only in thicker Martian crustal regions. Additionally, Na-rich feldspars suggest that there may be a source of water that can enter crustal material to induce partial melting at lower temperatures. Na and K-rich feldspars also suggest that the surface of Mars should not only have lava flows with Na- and Ca-containing feldspars, but also cones and lava domes where we find the evolved K-rich rocks. In the future, we will be looking for similar trends in other minerals, such as pyroxene, to infer Martian magma and surface compositions.

**Name:** Rose Harris

**Program:** UGS/Postbacc

**School:** Wheaton College- Massachusetts

**Group:** EES-14

**Mentor:** Roback, Robert Clifford

**Category:** Earth & Space Sciences

**Type:** Group Poster

**LA-UR:** 15-25485

# Sediment Particle Size Distribution from Core Holes of the LANL Chromium Plume

Between 1956 and 1972, between 31,000 and 72,000 kg of chromium used in laboratory cooling towers was released as effluent into Sandia Canyon. As a result, the aquifer underneath laboratory property is contaminated with high levels of chromium (VI), a toxin and carcinogen. Sampling groundwater monitoring wells on laboratory property provides information on the behavior of the chromium plume. For groundwater to enter a monitoring well, it must pass through a screen at the bottom. An optimal screen for these monitoring wells will allow groundwater to pass through while keeping out sediments. A particle size analysis of aquifer materials categorizes the subsurface material into sand, silt, or gravel. This information will help engineer better well screens and provide a better understanding of how water flows through the aquifer. Samples from five different core holes within the chromium plume were collected via sonic drilling at depths ranging from 732'-1125'. To obtain a particle size analysis, the samples were sieved into six different particle size fractions, of >4 mm, 2-4 mm, 1.4-2 mm, 0.355-1.4 mm, 180-355 µm, and smaller than 180 µm. The mass distributions were then plotted against their corresponding sieve size. The sample material was mostly from the Puye formation, a poorly sorted formation containing sedimentary rocks that have been pushed down from the Jemez volcanic field. The remaining samples were Miocene pumiceous, a poorly sorted pumice. The particle sizes were mostly silt, with some sands and gravels. The data demonstrated that there was a variety in sample material and size in the subsurface. The results of this study provide site-specific information in support of long-term monitoring well operations for chromium plume investigation and remediation.

**Name:** Coleman Kendrick

**Program:** HS COOP

**School:** Los Alamos High School

**Group:** XCP-2

**Mentor:** Robey, Bob

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** 15-25469

# Extrasolar Planetary Climate Model

A pseudo 3D extrasolar planet climate model is presented in which the ocean and atmosphere are simulated via stacked 2D meshes with a one dimensional vertical coupling. Both the ocean and atmosphere are simulated using a hydrodynamic solution, coupled to a simple thermodynamic ice model. Using coupled stacked 2D meshes, water evaporation, condensation, transport and other factors such as ice melting/formation and solar heating will be investigated. Currently, a standalone ice model is being investigated before coupling it with the 2D mesh model. Both a "0 layer" and "3 layer" ice model is developed which gives similar results to other ice models and measured data from the Arctic. For the standard Earth case, comparison model results are around 288 cm for a mean ice height whereas the developed 0 layer and 3 layer models give a mean ice thickness of 287.5 and 291.2 cm, respectively. Both models give a reasonable comparison to measured surface temperatures and other computed temperatures. When fully integrated, an extrasolar planet of different size, distance from host star, rotation period, orbital period, and ice/water content will be investigated.

**Name:** Alison Livesay

**Program:** GRA

**School:** University of Oklahoma-Norman

**Group:** ENV-ES

**Mentor:** Purtzer, LeAnn Carol

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** LA-UR 15-25478

# I Spy: Using Viewshed Analysis to Examine Rock Art on the Pajarito Plateau

Archaeologists working on the Pajarito plateau have proposed that petroglyph panels (rock art) functioned as “billboards” associating certain groups or clans with territories. We aim to test this assumption by answering the following questions. From where are these carved images visible? Are the vantage point many, few in number, or isolated near pueblo village sites? What other landmarks or built cultural features are visible from the panels themselves? Using a landscape perspective we investigate spatial relationships between sites and other prominent topological features, like peaks and springs. We selected rock art sites in Mortandad Canyon varying in placement on the landscape to determine whether petroglyphs were visible from multiple locations or were more restricted in their visibility. Presumably, smaller panels, not placed on the cliff face below the large residential pueblos, and less inter-visible, functioned as something other than billboards. Equally, panels with wide viewsheds or direct line of sight of prominent natural features might have functioned as shrines. Using Global Positioning Systems (GPS) units with sub-meter accuracy we took elevation points at each petroglyph panel, either on the cliff face below the mesa top or on boulders. This was then compared with digital elevation model (DEM) raster data acquired by a LIDAR flight in 2014. We conducted viewshed and line-of-sight analyses in ArcGIS, which was then tested by field visits with photography and a range finder to attempt to corroborate the computer generated results with the physical visual experience from different points on the landscape. Our results suggest that while some panels functioned as billboards, others have multiple or other discrete functions that were only meaningful to prehistoric inhabitants. This study’s importance lies in its use of Geographic Information Systems (GIS) applications as heuristic devices to explore interesting and dynamic social questions concerning everyday life in the past.

**Name:** Cody Smith

**Program:** UGS/Postbacc

**School:** St. John's College

**Group:** P-21

**Mentor:** Olinger, Chad Tracy

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25517

# SRIM Simulations to Understand Solar Wind Implantation

The Genesis Discovery Mission, launched 8/8/01, was designed to collect and return solar wind samples captured on the surfaces of ultra-pure materials. These samples would be used to measure solar composition and solar isotope abundances from four separate solar wind regimes. Bulk, which was exposed during the entire mission, CME, which was exposed during Coronal Mass Ejection Events, Fast, which was exposed during Coronal Hole Events and Slow, which was exposed to Interstream Solar Wind. On 9/8/04 the spacecraft returned but not as expected. A helicopter was meant to catch and lower it into a class 10 clean room. Instead, the return capsule did not deploy its parachute and crashed in Utah. The crash landing broke open the capsule contaminating the solar wind samples. To get the most information out of the remains of the Genesis project, SRIM (The Stopping and Range of Ions in Matter) is being used to simulate backscatter and implantation profiles. A Monte Carlo approach is being used to generate the input files. These simulated profiles are then used to correct the measured implant profile. Simulations are being performed to assist data interpretation in each combination of solar wind isotope, regime and target composition being measured by the international Genesis team.

**Name:** Lois Smith

**Program:** GRA

**School:** University of Michigan

**Group:** XCP-4

**Mentor:** Skoug, Ruth M

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25488

## Equatorial Noise Resonance with Low Energy Ions in RBSP HOPE and EMFISIS

After the discovery of the plasmaspheric post-midnight 1-10 eV ion loss between L =2 and L =3, we have expanded upon these results and connected the observed ion loss with changes in wave activity. Using the Van Allen Probes Helium, Oxygen, Proton, and Electron (HOPE) and the Electric and Magnetic Field Instrument Suite and Integrated Science (EMFISIS) instruments, we observed that changes in different frequency bands measured by EMFISIS are linked with changes in HOPE H+ thermal ion measurements. In particular, we examined changes in cyclotron heating and changes in Whistler wave activity at different MLTs, and we will present the results of this study.

**Name:** Sophie Stauffer

**Program:** GRA

**School:** University of New Mexico

**Group:** EES-14

**Mentor:** Rowland, Joel C

**Category:** Earth & Space Sciences

**Type:** Individual Poster

**LA-UR:** 15-25483

# Mapping River-Floodplain Sediment Exchange with Image Object Based Analysis

Sections of a river are said to reach equilibrium when the rates and areas of erosion equal those of deposition. Sediment transport strongly influences river channel structure, altering features such as channel width and depth, islands, and cutoffs. To understand the parameters governing sediment transport along a floodplain, we derived a method to determine areas of erosion and accretion from satellite imagery. Comparing changes in channel features through time and grouping areas of change by erosion or deposition, we identify locations that suggest strong floodplain and river interactions. An imbalance between erosion and accretion could indicate sediment is being stored along the floodplain. Determining the distribution of deposition along a floodplain typically involves field measurements, but in combination with this method we can provide an initial estimate of the volume of transported sediment. To begin our study, we generate river masks from Landsat imagery. The use of image object based analysis software (eCognition) has allowed us to utilize the full spectral values of the image to clearly delineate vegetated banks and the river. Image object based classification offers an improvement in the processing time over pixel based image analysis and provides a more automated method that can be executed on any global river for which images exist. We have generated river masks of several arctic rivers on a decadal time scale and have estimated areas of erosion and accretion. In addition to generating the masks, we are able to calculate channel width from the Landsat Images with a program called Spatially Continuous Riverbank Erosion and Accretion Measurements (SCREAM). Through this process we intend to gain a greater understanding of the river features that govern sediment transport, and ultimately sediment exchange between river and floodplain.

**Name:** Babatunde Adigun

**Program:** GRA

**School:** Imperial College London

**Group:** NEN-5

**Mentor:** Fensin, Michael Lorne

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** 15-25545

# Reactor Modeling for Nonproliferation Safeguards

Here we model and present the initial results of burnup dependent aspects of gas cooled reactors. Beginning with legacy British gas-cooled reactors, we look at how certain common assumptions in reactor modeling ultimately affect the isotopics of the reactor. The study on the assumptions included sensitivity analyses on clad thickness, and fuel and moderator density. Delving further, we also examine the effect on burnup, of burning with a critical spectra with control rods inserted versus a non-critical spectra without control rods. This will help in our ultimate objective of determining if past simplified models are plausible approximations compared to more detailed core models.

**Name:** Leyla Akhadov

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** B-10

**Mentor:** Harris, Jennifer Foster

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25529

## Microfluidic Method to Determine Elastic Properties of Flexible Membranes

Artificial lungs grown in a laboratory from human cells are becoming increasingly important to the medical community because of their use in drug testing. However, for the cells to function as they would in a healthy, human lung, they must be inflated and deflated as they would be in a breathing lung. To simulate this, the cells can be grown on a flexible membrane that inflates and deflates as a lung would. Unfortunately, a major problem with the production and development of these membranes is the difficulty that comes along with quantifying the characteristics of the membrane. Current technologies for measuring a membrane's thickness and elasticity, such as atomic force microscopy, are expensive and require extensive training to perform. The elastic modulus, the ratio of the stress applied to the membrane and the resulting strain on the membrane, is perhaps its most important feature; additionally, it can straightforwardly be calculated given the pressure applied to the membrane and the resulting change in volume of the membrane. Taking advantage of these features of the Young's Modulus calculation allowed us to create a microfluidics device that lets the user easily observe the change in volume that follows a specific change in pressure. Here, the change in volume under the membrane after a prescribed pressure change is measured by the displacement of a colored liquid, in a simplified and more accurate translation of the classic Bulge Test. The device itself is simple, inexpensive, and easily assembled, lending itself to use by a wide range of people, and will eventually lead to more widespread use of synthetic membranes.

**Name:** Adam Allevato

**Program:** GRA

**School:** UT Austin

**Group:** DET-2

**Mentor:**

**Category:** Engineering

**Type:** Group Poster

**LA-UR:** LA-UR-15-25056

# Robotic Automation Design for Detonator Component Metrology

As part of the manufacturing process, Detonator Product Realization (DET-2) performs lot acceptance testing to ensure that detonator components meet numerous design tolerances. The current testing method is destructive and time-consuming, as parts must be cross-sectioned (cut in half) to be measured accurately. The goal of this project is to replace the cross-section operation with computed tomography (CT) scans and automatic tolerance verification. We present three techniques for further automating these CT scans, resulting in improved production efficiency and improved worker productivity. First, we present the design of a multipart fixture that will allow many parts to be loaded into the CT scanner simultaneously. Second, we demonstrate the integration of hardware and software framework designed to automatically load and unload these fixtures into the CT scanner using a Motoman SIA5 7-degree of freedom robotic arm. Finally, we have developed techniques for robotically loading the fixtures with detonator components. We demonstrate that together, these three process improvements will results in significant time savings during detonator component inspection.

**Name:** Robert Anderson

**Program:** GRA

**School:** The University of Texas at Austin

**Group:** MET-2

**Mentor:** Gubernatis, Dave

**Category:** Engineering

**Type:** Group Poster

**LA-UR:** LA-UR-15-25727

# Mobile Robotic Automation of Non-Contact Nuclear Material Operations at TA-55

In order to increase safety and reduce the radiation dosage to personnel in mission-critical nuclear activities at the laboratory, new robotic systems must be developed to accomplish tasks currently performed by human workers. To this end, the laboratory is working in conjunction with the Nuclear Robotics Group at the University of Texas at Austin to design and deploy a mobile platform for service in the Plutonium Facility at TA-55. The primary mission of the system is to transport containers of hazardous nuclear material, including plutonium, to and from the PF-4 nuclear material vault. However, a crucial component for the integration of autonomous systems into mission critical areas is user comfort; all personnel involved must be able to work safely around the system and must be confident in its ability to accomplish its given tasks. Therefore, two intermediate non-contact systems are currently in development on-site at LANL in order to increase familiarity and prove an array of valuable non-contact capabilities, before proceeding with contact task integration. These additional capabilities include: autonomous inventory of material, routine radiation and criticality surveying, and security monitoring. The Adept PioneerLX features a robust and reliable navigation and localization suite using Monte-Carlo localization. It also features an array of sensors ensuring safe autonomous operation around personnel, including LIDAR and SONAR vision sensors and emergency physical contact bumper switches. The platform is able to support an array of additional sensors and actuators as well, including RGB-D cameras for barcode recognition and radiation survey instruments such as alpha detectors. Barcode recognition allows the system to identify the presence and exact 3D pose of labeled objects, providing for robust inventory management Software is continuously being developed to integrate all of these sensing and navigation capabilities into a cohesive, user-friendly environment allowing for either tele-operative or autonomous operation of complex tasks.

**Name:** Krishan Bhakta

**Program:** UGS/Postbacc

**School:** New Mexico Tech

**Group:** IPM

**Mentor:** Eglin, Judith Lynne

**Category:** Engineering

**Type:** Group Poster

**LA-UR:**

# Fire Suppression System Testing Within a Closed Glovebox

Various dry chemical fire suppression systems are being considered for installation in gloveboxes. They are typically engineered systems with requirements based on the volume of the enclosure, combustible material, air flow rate, etc. Fire tests will be performed to evaluate tar the efficacy of selected fire suppression systems. The maximum airflow rate and minimum allowable working pressures for a working glovebox will be utilized as bounding criteria for fire tests to yield the most conservative and comprehensive fire test plan to suit Los Alamos National Labs (LANL) requirements.

**Name:** John Bilberry

**Program:** UGS/Postbacc

**School:** University of Texas at El Paso

**Group:** CCS-3

**Mentor:** Toole, Gasper Loren

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25042

# Creating an Open Access National Electric Grid Model

There is a recognized need for open access energy grid data to be used in the Emergency Management and Response (EMR) field, as well as unrestricted grid models for the purpose of research and simulation. Proprietary grid models are costly to prepare and are severely restricted in applications to EMR. Licensing and other restrictions are problematic for use in research and simulation fields. Is it possible to construct a model of the US electric grid using strictly public and openly available information? To address this problem an open access US grid data set has been constructed. From this data set an executable power flow model, that simulates the flow of electricity on the US electrical grid, will be constructed. To accomplish this task, first the network topology will be verified. Geo location and verification of electrical substations and transmission lines will be accomplished through a variety of techniques including openly available documents as well as satellite imagery analysis. Once the network topology has been verified, the construction of an executable power flow model will begin. To construct the executable model, known characteristics of line and node features will be added as network attributes. Next using a set of state-of-art tools as well as developing inferenced heuristic rule sets, the remaining network properties will be estimated. The model results will then be tested and compared to existing known solutions for accuracy. The main outcome of this project is the creation of a national grid data set that is sharable across all levels of government. This will allow advancements in grid research by providing more accessible models and data sets for research and simulation. Additionally an unrestricted grid data set will be available to the Emergency Management and Response community.

**Name:** Hanah Choice

**Program:** UGS/Postbacc

**School:** University of Texas at Austin

**Group:** NPI-2

**Mentor:** Vaidya, Raj

**Category:** Engineering

**Type:** Group Poster

**LA-UR:** 15-25262

# Robotic Applications in Plutonium Science and Manufacturing Support

Los Alamos National Laboratory (LANL) supports a variety of radioactive materials research initiatives. It is imperative from a safety perspective to investigate technologies that limit worker exposure and improve operations reliability. To achieve these end goals, smart computing concepts such as goal-oriented action programming and holistic component integration will be used. The system being considered consists of several main components: the Adept Pioneer LX mobile platform, a custom-built Schunk LWA Powerball robotic arm, and a PEH 30 electric gripper. The Pioneer LX provides sonar, a 270° laser rangefinder, and physical contact sensors for safety and localization purposes. A neutron detector will be mounted upon this platform, providing real-time radiation monitoring capabilities. The robot is being programmed in C++ using ROS packages to synchronize its components. The integrated robotic system being studied will monitor the locations and integrity of storage containers. It will also be able to organize and retrieve them when necessary. Should an uncontrolled or unsafe situation develop, the robot could gather technical data and secure the area, preventing excessive exposure to RCT's. Automation of these tasks will increase worker safety, improve manufacturing reliability, and eventually decrease operational costs. The robot is being developed for initial on-site testing by late fall 2015.

**Name:** **Matthew Davenport**

**Program:** **UGS/Postbacc**

**School:** **New Mexico Institute of Mining and Technology**

**Group:** **NPI-2**

**Mentor:** **Vaidya, Raj**

**Category:** **Engineering**

**Type:** **Group Poster**

**LA-UR:** **15-25262**

# Robotic Applications in Plutonium Science and Manufacturing

Los Alamos National Laboratory (LANL) supports a variety of radioactive materials research initiatives as part of the programs completed at TA-55. Actinide processing capabilities at LANL are critical in completing these mission deliverables. It is imperative from a safety perspective to investigate technologies that limit worker exposure and improve operations reliability. Robotic solutions offer unparalleled potential for repeatability, efficiency, and worker safety. However, most industrial robots rely upon remote tele-operation or utilize restrictive programming routines. To achieve these end goals, smart computing concepts such as goal-oriented action programming and holistic component integration are being investigated in order to achieve almost total system automation. The system being considered consists of several main components: the Adept Pioneer LX mobile platform, a custom-built Schunk LWA Powerball robotic arm, and a PEH 30 electric gripper. The Pioneer LX provides sonar, a 270° laser rangefinder, and physical contact sensors for safety and localization purposes. A neutron detector will be mounted upon this platform, providing real-time radiation monitoring capabilities. The robot is being programmed in C++ using ROS packages to synchronize its components. This combination of sensors and payload delivery capabilities will be used to bolster the resources of Radiation Control Technicians (RCT's) within LANL's nuclear material vault. The integrated robotic system being studied will monitor the locations and integrity of storage containers. It will also be able to organize and retrieve them when necessary. Should an uncontrolled or unsafe situation develop, the robot could gather technical data and secure the area, preventing excessive exposure to RCT's. This technology has the potential for broader application, such as glovebox-contained manufacturing and chemical processing. Automation of these tasks will increase worker safety, improve manufacturing reliability, and eventually decrease operational costs. The robot is being developed for initial on-site testing by late fall 2015.

**Name:** Narendra De

**Program:** GRA

**School:** Purdue University

**Group:** M-7

**Mentor:** Tappan, Bryce C

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** 15-21930

# Engineering a Novel Solid Rocket Propulsion System

Current solid propellant systems have proven reliable over the decades but have long since reached their limit in terms of achievable system safety and performance. Despite this, the US DoD, NASA and commercial organizations continue to request increasingly higher-energy systems with an increased level of safety. The demand for safer systems is becoming more relevant with the recent boom in commercial space endeavors, particularly when considering space tourism. This safety consideration has brought forth a revival in solid fuel/liquid oxidizer hybrid rockets, despite the inherent problems of these systems such as low mass-burning rates requiring large surface areas in the fuel section to achieve the same thrust as solid propellants. The two characteristics of increased safety and higher performance, however, are almost always mutually exclusive, being that typically the higher energy systems almost always have the penalty of being higher hazard. The aim of the proposed effort is to develop a segregated fuel/oxidizer propellant system that would be a major break-though in solid rocket propulsion in terms of safety and energy. The proposed system is a combination of novel materials that allow for a radically new engineering design. Because of the development of high-nitrogen/high hydrogen energetics at LANL that contain little or no oxygen, a segregated tandem system can be designed such that the burning energetic materials will provide fuel from their decomposition that will be oxidized in a separate chamber by reaction with a solid oxidizer. Because the fuel and the oxidizer will remain separated until combustion of the fuel is initiated, and are both are relatively (or completely) insensitive to shock, the chance of accidental detonation or initiation of the rocket is dramatically reduced. This provides an unprecedented level of safety, opening up previously inaccessible utilization of higher energy components, thereby exceeding performance of state-of-the-art solid propellants.

**Name:** Benjamin Ebersole

**Program:** GRA

**School:** University of Texas at Austin

**Group:** MET-2

**Mentor:** Gubernatis, Dave

**Category:** Engineering

**Type:** Group Poster

**LA-UR:** LA-UR-15-25727

# Mobile Robotic Automation of Non-Contact Nuclear Material Operations at TA-55

In order to increase safety and reduce the radiation dosage to personnel in mission-critical nuclear activities at the laboratory, new robotic systems must be developed to accomplish tasks currently performed by human workers. To this end, the laboratory is working in conjunction with the Nuclear Robotics Group at the University of Texas at Austin to design and deploy a mobile platform for service in the Plutonium Facility at TA-55. The primary mission of the system is to transport containers of hazardous nuclear material, including plutonium, to and from the PF-4 nuclear material vault. However, a crucial component for the integration of autonomous systems into mission critical areas is user comfort; all personnel involved must be able to work safely around the system and must be confident in its ability to accomplish its given tasks. Therefore, two intermediate non-contact systems are currently in development on-site at LANL in order to increase familiarity and prove an array of valuable non-contact capabilities, before proceeding with contact task integration. These additional capabilities include: autonomous inventory of material, routine radiation and criticality surveying, and security monitoring. The Adept PioneerLX features a robust and reliable navigation and localization suite using Monte-Carlo localization. It also features an array of sensors ensuring safe autonomous operation around personnel, including LIDAR and SONAR vision sensors and emergency physical contact bumper switches. The platform is able to support an array of additional sensors and actuators as well, including RGB-D cameras for barcode recognition and radiation survey instruments such as alpha detectors. Barcode recognition allows the system to identify the presence and exact 3D pose of labeled objects, providing for robust inventory management Software is continuously being developed to integrate all of these sensing and navigation capabilities into a cohesive, user-friendly environment allowing for either tele-operative or autonomous operation of complex tasks.

**Name:** Shuprio Ghosh

**Program:** UGS/Postbacc

**School:** Santa Fe Community College

**Group:** MPA-CINT

**Mentor:** Azad, Abul

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** 15-25528

# Cost Reduction of Algal Biofuel Production – Why Not Start at the Laboratory?

Based on the 2013 multi-year program report from the Department of energy's Bioenergy technologies office, algae cultivation cost must be reduced by ~4 times by 2022 to make Algal biofuel competitive. Algal biofuel research community is taking significant initiatives from different perspectives to address this challenge. We believe the cost reduction should start at the bottom of the chain, at the laboratory. Therefore, our goal was to study a new bioreactor system that is low cost, safe, and environment friendly. Furthermore, we intend to replace traditional shakers in the laboratory saving 100% of their operating cost with electricity. Usually, it is often overlooked that our traditional shakers consume electricity 24 hours a day for operation, produce noise, and take up space. To address this problem, we investigated a miniaturized air-lift bioreactor design for algae research laboratory applications. In our bioreactor two concentric rectangular tubes are arranged in such a way that when air bubbles pass through the inner tube, it creates a circulation inside the bioreactor preventing the algae from settling due to gravity. Growth characteristics for four different algae strains (Chlorella sorokiniana, Picochlorum, Synechocystis 6803, and Tetraselmis striata) were studied for two weeks to validate the bioreactors. Optical density was used to measure the growth rate. The study showed satisfactory growth of algae in the bioreactors. Each bioreactor can hold 55-65 mL of culture. It is possible to house 12-18 bioreactors within 1 square foot of surface space. No electricity is required to get the circulation with in the bioreactors. Our demonstration of successful algae growth within these bioreactors have the potential to become an essential tool for laboratory based algal biofuel research.

**Name:** John Gibson

**Program:** UGS/Postbacc

**School:** New Mexico Institute of Mining and Technology

**Group:** W-6

**Mentor:** Sanchez, Nate

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25625

# Solder vs. Conductive Epoxy in Chip Slapper Detonators

In order to analyze the effects of Conductive epoxy versus solder in the conductive joints of a Chip Slapper Detonator with respect to function time and threshold function voltage components in the detonation process, a series of tests were developed and conducted at varying voltages to illustrate the shock wave propagation emitted over time by the slapper system. Both Hardfire and Neyer tests were conducted in order to establish a direct and accurate comparison between solder and conductive epoxy. Neyer testing is based off of the Barry T. Neyer program calculating the threshold voltage needed to initiate detonation in a given system. For these test series we chose to use a chip slapper detonator in conjunction with a PETN explosive pellet of 1.65 g/cm$^3$ compressed density, initiated by a LANL TSD fire set. Using a digital streak camera we were able to obtain high resolution streak images of the detonation process and evaluate the precise timing of the breakout and center of initiation, using a MATLAB Graphical User Interface (GUI) code developed by W-6. Upon the results of the test there will be a follow up analysis of solder in other procedures such as Thermal Cycling, shear strength testing and 3 axis sustained vibration to determine resilience to external and elemental factors.

Name: Mark Graham

Program: UGS/Postbacc

School: New Mexico Institute of Mining and Technology

Group: MET-1

Mentor: Schollenberger, Timothy

Category: Engineering

Type: Individual Poster

LA-UR: 15-25497

# Tool and Fixture Design

In a manufacturing process, a need is identified and a product is created to fill this need. While design and engineering of the final product is important, the tools and fixtures that aid in the creation of the final product are just as important, if not more so. Power supplies assembled at the TA-55 PF-5 have been designed by an excellent engineering team. The task in PF-5 now is to ensure that all steps of the assembly and manufacturing process can be completed safely, reliably, and in a quality repeatable manner. One of these process steps involves soldering fine wires to an electrical connector. During the process development phase, the method of soldering included placing the power supply in a vice in order to manipulate it into a position conducive to soldering. This method is unacceptable from a reliability, repeatability, and ergonomic standpoint. To combat these issues, a fixture was designed to replace the current method. To do so, a twelve step engineering design process was used to create the fixture that would provide a solution to a multitude of problems, and increase the safety and efficiency of production.

**Name:** Angus Guider

**Program:** UGS/Postbacc

**School:** Rochester Institute of Technology

**Group:** NPI-2

**Mentor:** Vaidya, Raj

**Category:** Engineering

**Type:** Group Poster

**LA-UR:** 15-25262

# Robotic Applications in Plutonium Science and Manufacturing

Los Alamos National Laboratory (LANL) supports a variety of radioactive materials research initiatives as part of the programs completed at TA-55. Actinide processing capabilities at LANL are critical in completing these mission deliverables. It is imperative from a safety perspective to investigate technologies that limit worker exposure and improve operations reliability. Robotic solutions offer unparalleled potential for repeatability, efficiency, and worker safety. However, most industrial robots rely upon remote tele-operation or utilize restrictive programming routines. To achieve these end goals, smart computing concepts such as goal-oriented action programming and holistic component integration are being investigated in order to achieve almost total system automation. The system being considered consists of several main components: the Adept Pioneer LX mobile platform, a custom-built Schunk LWA Powerball robotic arm, and a PEH 30 electric gripper. The Pioneer LX provides sonar, a 270° laser rangefinder, and physical contact sensors for safety and localization purposes. A neutron detector will be mounted upon this platform, providing real-time radiation monitoring capabilities. The robot is being programmed in C++ using ROS packages to synchronize its components. This combination of sensors and payload delivery capabilities will be used to bolster the resources of Radiation Control Technicians (RCT's) within LANL's nuclear material vault. The integrated robotic system being studied will monitor the locations and integrity of storage containers. It will also be able to organize and retrieve them when necessary. Should an uncontrolled or unsafe situation develop, the robot could gather technical data and secure the area, preventing excessive exposure to RCT's. This technology has the potential for broader application, such as glovebox-contained manufacturing and chemical processing. Automation of these tasks will increase worker safety, improve manufacturing reliability, and eventually decrease operational costs. The robot is being developed for initial on-site testing by late fall 2015.

**Name:** Nicholas Hashem

**Program:** UGS/Postbacc

**School:** UT Austin

**Group:** DET-2

**Mentor:** Armijo, Mark A ;

**Category:** Engineering

**Type:** Group Poster

**LA-UR:** LA-UR-15-25056

# Robotic Automation Design for Detonator Component Metrology

As part of the manufacturing process, Detonator Product Realization (DET-2) performs lot acceptance testing to ensure that detonator components meet numerous design tolerances. The current testing method is destructive and time-consuming, as parts must be cross-sectioned (cut in half) to be measured accurately. The goal of this project is to replace the cross-section operation with computed tomography (CT) scans and automatic tolerance verification. We present three techniques for further automating these CT scans, resulting in improved production efficiency and improved worker productivity. First, we present the design of a multipart fixture that will allow many parts to be loaded into the CT scanner simultaneously. Second, we demonstrate the integration of hardware and software framework designed to automatically load and unload these fixtures into the CT scanner using a Motoman SIA5 7-degree of freedom robotic arm. Finally, we have developed techniques for robotically loading the fixtures with detonator components. We demonstrate that together, these three process improvements will results in significant time savings during detonator component inspection.

**Name:** Fritz Hieb

**Program:** GRA

**School:** New Mexico Tech

**Group:** IPM

**Mentor:** Eglin, Judith Lynne

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:**

# Water Intrusion Effects for Glovebox Gloves

Water-based fire suppression systems can be utilized to extinguish unexpected fires inside a glovebox enclosure. The deployment of a water-based fire suppression system can place significant stress on the glovebox and associated components. The goal of this work was to quantitatively measure the response of a glovebox system to water intrusion that might occur during fire suppression. Specific attention was given to the effect of the water intrusion on three types of glove box gloves as well as their stored state clamped vs. unclamped). Significant deformation was observed in all types of gloves tested, with many failing when the water column reached the upper limits of the glovebox interior.

**Name:** Matthew Horn

**Program:** GRA

**School:** University of Texas at Austin

**Group:** NPI-2

**Mentor:** Vaidya, Raj

**Category:** Engineering

**Type:** Group Poster

**LA-UR:** 15-25262

# Robotic Applications in Plutonium Science and Manufacturing

Los Alamos National Laboratory (LANL) supports a variety of radioactive materials research initiatives as part of the programs completed at TA-55. Actinide processing capabilities at LANL are critical in completing these mission deliverables. It is imperative from a safety perspective to investigate technologies that limit worker exposure and improve operations reliability. Robotic solutions offer unparalleled potential for repeatability, efficiency, and worker safety. However, most industrial robots rely upon remote tele-operation or utilize restrictive programming routines. To achieve these end goals, smart computing concepts such as goal-oriented action programming and holistic component integration are being investigated in order to achieve almost total system automation. The system being considered consists of several main components: the Adept Pioneer LX mobile platform, a custom-built Schunk LWA Powerball robotic arm, and a PEH 30 electric gripper. The Pioneer LX provides sonar, a 270° laser rangefinder, and physical contact sensors for safety and localization purposes. A neutron detector will be mounted upon this platform, providing real-time radiation monitoring capabilities. The robot is being programmed in C++ using ROS packages to synchronize its components. This combination of sensors and payload delivery capabilities will be used to bolster the resources of Radiation Control Technicians (RCT's) within LANL's nuclear material vault. The integrated robotic system being studied will monitor the locations and integrity of storage containers. It will also be able to organize and retrieve them when necessary. Should an uncontrolled or unsafe situation develop, the robot could gather technical data and secure the area, preventing excessive exposure to RCT's. This technology has the potential for broader application, such as glovebox-contained manufacturing and chemical processing. Automation of these tasks will increase worker safety, improve manufacturing reliability, and eventually decrease operational costs. The robot is being developed for initial on-site testing by late fall 2015.

**Name:** Ryan Leon

**Program:** UGS/Postbacc

**School:** University of Michigan

**Group:** MST-16

**Mentor:** Saleh, Tarik A.

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** 15-21776

# CNC Tooling Development for Plutonium Machining in Gloveboxes

Machining plutonium can be expensive due to equipment installation, complications of glovebox use, and personnel training. Enclosed CNC mill and lathe tools that are small enough to fit into a glovebox intro hood and out through bagout ports will make specimen fabrication easier, faster, safer and cheaper. This talk describes ongoing work in development of modular inexpensive machining capabilities for glovebox use. Once installed, an operator's user inputs are translated into G-code automated tooling paths, removing the operator from harm's way during the cutting. The polycarbonate enclosure improves material accountability and safety by reducing chip spread and adding an extra barrier for potential sharps or thrown tools. The system has DC brushless motors and ergonomic adaptations for an inert glovebox environment. These advantages will help yield more samples for experiments in large scale plutonium science campaigns as well as lowering the barrier for researchers to conduct smaller scale investigations.

**Name:** Andrew Matejunas

**Program:** GRA

**School:** New Mexico Tech

**Group:** IPM

**Mentor:** Eglin, Judith Lynne

**Category:** Engineering

**Type:** Group Poster

**LA-UR:**

# Fire Suppression System Testing Within a Closed Glovebox

Various dry chemical fire suppression systems are being considered for installation in gloveboxes. They are typically engineered systems with requirements based on the volume of the enclosure, combustible material, air flow rate, etc. Fire tests will be performed to evaluate tar the efficacy of selected fire suppression systems. The maximum airflow rate and minimum allowable working pressures for a working glovebox will be utilized as bounding criteria for fire tests to yield the most conservative and comprehensive fire test plan to suit Los Alamos National Labs (LANL) requirements.

**Name:** Christopher McGahee

**Program:** UGS/Postbacc

**School:** Pennsylvania State University

**Group:** NEN-1

**Mentor:** Henzl, Vladimir

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** 15-25662

# Random Neutron Contribution to Simulation of Pulse Train for Correlated Counting

To assure good accountability and prevent proliferation of special nuclear material (SNM), nuclear safeguards typically employs 3He based thermal neutron detection systems to detect fission signatures. These systems are composed of a set of neutron detectors which can detect multiple neutrons released from a single spontaneous fission event. One of the key tools to determine the quantity of SNM being measured is neutron coincidence and multiplicity counting. Of importance to coincidence and multiplicity measurements is the appropriate correction of dead time of the system, as correlated neutron events from nuclear fissions are affected by dead time in a different manner than random neutron events typically assumed in dead time corrections. If this dead time is not properly characterized and corrected, then the accuracy of a measurement and the quantity of SNM being measured can be adversely affected. To properly characterize the dead time, realistic simulations are necessary especially for areas not easily accessible by experimental measurements. Existing simulations, however, account for the neutron production from spontaneous fissions but not for the random neutron contribution from (α, n) reactions that may occur in certain compounds like plutonium oxide (PuO2), plutonium fluoride (PuF4), or in compounds with different impurities. This contribution needs to be taken into account to assure realistic characteristics of the simulated neutron detections. For this project, the (α, n) reactions were modeled for the Epithermal Neutron Multiplicity Counter (ENMC) detection system using MCNP 6.11. The simulation results including spontaneous fissions as well as the (α, n) reaction contributions were compared with experimental data to determine the effect of (α, n) reactions on dead time of the system. The dead time response determined from these comparisons will be used to benchmark and update the existing dead time models for this and other multiplicity and coincidence systems.

**Name:** Jeffrey Nguyen

**Program:** GRA

**School:** Colorado State University

**Group:** AOT-IC

**Mentor:** Sedillo, James Daniel

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25633

# Pre-Conceptual Design for the Isotope Production Facility Adjustable Collimator

The pre-conceptual design for the variable aperture collimation system for the Isotope Production Facility (IPF) at Los Alamos Neutron Science Center (LANSCE) is described. The adjustable aperture accommodates different targets and production objectives. The collimator consists of four graphite plates designed to absorb fringe particles that would otherwise damage the IPF target window further downstream. The collimator will be exposed to 41, 72, and 100 MeV proton beam. The physics of beam on collimator interactions and the plan for further work is described.

**Name:** Logan Ott

**Program:** UGS/Postbacc

**School:** Fort Lewis College

**Group:** ISR-5

**Mentor:** Storms, Steven Alexander

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25535

# Targeted Atmospheric Chemistry Observations from Space

Increased living standards in the developing world are creating a need for enhanced air quality and pollution monitoring systems. Observing local emission patterns, pollutant propagation, and understanding their effects on air quality and climate will be essential for treaty monitoring and to inform policies as more and more countries prioritize environmental issues. Existing pollution monitoring systems have limited targeting capabilities, and certain parts of the globe lack significant monitoring at all. NASA has solicited a series of Earth Venture missions to address these issues and to revitalize our nation's satellite network for Earth systems science. In response to these demands, LANL scientists and engineers are proposing CubeSat-based pollution monitoring techniques with unprecedented geographic coverage, spatial resolution, and revisit time. CubeSats are a new class of miniature satellites, which through reduced cost, have potential to make space missions available to a broader community. Having successfully operated 12 communications CubeSats in Low Earth Orbit, LANL is a world leader in CubeSat technology. Prometheus Block 2 is the current generation under development at LANL and will have capacity to host scientific payloads. For pollution monitoring, the proposed payload is a UV-VIS spectrometer optimized to detect atmospheric $NO_2$, $SO_2$, absorbing aerosols, and ozone. LANL-developed CubeSat attitude control technologies will allow precise targeting/tracking of pollution hotspots, and the low cost makes it feasible to deploy a constellation of 10+ CubeSats around the globe for large geographic coverage and frequent re-visit times.

**Name:** Abel Raymer

**Program:** GRA

**School:** North Carolina A&T State University

**Group:** P-24

**Mentor:** Fernandez, Juan Carlos

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25767

# Target Holder

Acceleration of charged particles as they interact with “collisionless shocks” is a widespread phenomenon occurring across the entire universe. Unlike the well-known collisional hydrodynamic shocks, in the collisionless shocks the particle collision time is much larger than the particle transit time through the shock. This astrophysical phenomenon occurs regularly in the cosmos, for example, at supernova shocks, during fast coronal mass ejection from the sun forming solar-wind shocks and at the planetary bow shocks. A particular type of electromagnetic plasma instability known as Weibel instability is believed to be the dominant mechanism behind the formation of these collisionless shocks in the cosmos. Weibel instability leads to an exponentially growing magnetic field arising from the electromagnetic micro turbulences in initially un-magnetized or weakly magnetized plasmas present in the vicinity of gamma ray burst sources, supernovae and galactic cosmic rays. How these magnetic fields are generated and what are their structures, which dissipation mechanism is dominant, which physical processes lead to shock formation, and how particles are accelerated in these shocks remain open questions. Apart from indirect spacecraft observations, there is no direct observation to date of collisionless shocks mediated by Weibel instability. Experimental preparations are underway at LANL Trident laser facility to probe Weibel instability mediated collisionless shocks using two ultra-intense laser pulses in a pump-probe configuration. We have designed a special target holder that can accommodate two targets in close proximity for this specific experiment.

**Name:** Jonathon Salazar

**Program:** UGS/Postbacc

**School:** New Mexico Tech

**Group:** IPM

**Mentor:** Eglin, Judith Lynne

**Category:** Engineering

**Type:** Group Poster

**LA-UR:**

## Fire Suppression System Testing Within a Closed Glovebox

Various dry chemical fire suppression systems are being considered for installation in gloveboxes. They are typically engineered systems with requirements based on the volume of the enclosure, combustible material, air flow rate, etc. Fire tests will be performed to evaluate tar the efficacy of selected fire suppression systems. The maximum airflow rate and minimum allowable working pressures for a working glovebox will be utilized as bounding criteria for fire tests to yield the most conservative and comprehensive fire test plan to suit Los Alamos National Labs (LANL) requirements.

**Name:** Christopher Sanchez

**Program:** UGS/Postbacc

**School:** New Mexico Tech

**Group:** IPM

**Mentor:** Eglin, Judith Lynne

**Category:** Engineering

**Type:** Group Poster

**LA-UR:**

# Fire Suppression System Testing Within a Closed Glovebox

Various dry chemical fire suppression systems are being considered for installation in gloveboxes. They are typically engineered systems with requirements based on the volume of the enclosure, combustible material, air flow rate, etc. Fire tests will be performed to evaluate tar the efficacy of selected fire suppression systems. The maximum airflow rate and minimum allowable working pressures for a working glovebox will be utilized as bounding criteria for fire tests to yield the most conservative and comprehensive fire test plan to suit Los Alamos National Labs (LANL) requirements.

**Name:** Lexey Sbriglia

**Program:** UGS/Postbacc

**School:** University of Nevada- Reno

**Group:** AET-1

**Mentor:** Wachtor, Adam Joseph

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** 15-25244

# Embedding Sensors in FDM Plastic Parts During Additive Manufacturing

For parts built through the layer by layer material deposition process of additive manufacturing (AM), it is essential to qualify both the material and geometrical characteristics of the fabricated part to ensure reproducibility of the printing process. Open source fused deposition modeling (FDM) machines provide users with a broad set of parameters to control the build process. This work evaluates the effects on the aforementioned characteristics caused by operator choices, such as filament type, print speed, nozzle and bed temperatures, layer thickness, or building in a thermally controlled or fully open environment. Integrated circuit piezoelectric accelerometers were embedded into the parts during the build process, and modal analyses of the parts was then carried out using an electrodynamic shaker. An eigenvalue solution for the natural frequencies of an ideal part with homogenous material properties was solved for using SolidWorks Simulation and used as a benchmark against the experimental measurements of the FDM parts.

**Name:** Andrew Sharp

**Program:** GRA

**School:** The University of Texas at Austin

**Group:** MET-2

**Mentor:** Gubernatis, Dave

**Category:** Engineering

**Type:** Group Poster

**LA-UR:** LA-UR-15-25661

# Software Frameworks for Contact and Non-contact Robotic Arm Tasks

When working with nuclear materials, it can sometimes be difficult to protect the worker from larger doses or injuries from environmental hazards, even with stringent procedural and engineering controls in place. For example, some nuclear processes require glovebox work in close proximity to radioactive and mechanical hazards. Working in glovebox gloves can limit dexterity and increase the chance for an ergonomic injury due to constrained and/or repetitive movement. It may be possible to eliminate most hazards with the use of robotic manipulators. For this reason, the laboratory is working with the Nuclear Robotics Group at the University of Texas at Austin to develop industrial robotic manipulator controls to perform some TA-55 Plutonium Facility (PF-4) tasks which are currently completed manually by radiation workers. There are a wide variety of applications where robotic manipulation could be implemented at PF-4. These applications can be split into two broad task categories: contact and non-contact tasks. The first category includes tasks where the robot needs to make contact with the environment, such as assembly, disassembly, or packaging. Non-contact tasks include radiological surveys, storage inventory, and inventory visual inspection. This poster presents work being done in both categories which could have applications in a large number of processes at PF-4. When working on non-contact tasks, it is often difficult to ensure predictable movement of a robotic manipulator in an unknown environment. Toward this end, a Descartes path planner application is being developed for smooth motion with minimized joint reconfigurations. Contact task controllers are often built for very specific applications and are not always easily extended to multiple tasks. To make the use of robotics for contact tasks at PF-4 more feasible, a general contact task controller that can be configured for many simple contact tasks is also being developed.

**Name:** Megan Smith

**Program:** GRA

**School:** North Carolina State University

**Group:** AET-2

**Mentor:** Davis, Adam Christopher

**Category:** Engineering

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25597

# Sensitivity Study of Void Coefficients in the SHEBA-II reactor using MCNP6

The purpose of this study is to investigate the effects of void volumes, void locations, and temperature on the critical solution height of the SHEBA-II reactor. This investigation involves the use of MCNP6 and its utility, mcnp_pstudy, to model the SHEBA-II reactor. Four void locations were analyzed with volumes ranging from 374.7848 cm3 to 436.4586 cm3. Two of the void locations were located along the inner thimble of the reactor. One of these inner voids was positioned so that the bottom of the void was at half of the critical solution height (calculated with no voids present), and the second inner void was positioned at the bottom of the reactor. The two outer voids were located along the walls of the tank containing the solution with the same two vertical positions as the inner voids. A temperature analysis was then performed for these varying positions and volumes. The temperature ranged from room temperature to just above the boiling point of the solution (Uranyl Fluoride). The results were converted to a usable csv file using FORTRAN, and MATLAB was used to visualize the data in the csv file.

Name: Lynette Torrez
Program: UGS/Postbacc
School: University of New Mexico
Group: MPA-CMMS
Mentor: Nguyen, Doan Ngoc
Category: Engineering
Type: Individual Poster
LA-UR: LA-UR-15-25653

## Electromagnetic Interaction between Insert & Outsert Coils of 100T Magnet System

The multishot 100 Tesla magnet at the Pulsed Field Facility of LANL consists of an insert 60T coil powered by a capacitor placed in a 40T outsert magnet powered by a 1.4 Gigawatt Generator. The outsert magnet consists of 7 individual concentric coils configured into three coil-groups. In many cases, only the Insert is fired, causing induced voltage on the outsert coils. We use FEM (Finite Element Method) simulation implemented in COMSOL Multiphysics software to understand the electromagnetic interaction between the insert and outsert coil-group. This study will allow us to predict and avoid the overloaded induced voltage on the outsert coil when the insert is fired.

**Name:** Rusty von Sternberg

**Program:** GRA

**School:** The University of Texas at Austin

**Group:** MET-1

**Mentor:** Williams, Joshua Murry

**Category:** Engineering

**Type:** Group Poster

**LA-UR:** LA-UR-15-25661

# Software Frameworks for Contact and Non-contact Robotic Arm Tasks

When working with nuclear materials, it can sometimes be difficult to protect the worker from larger doses or injuries from environmental hazards, even with stringent procedural and engineering controls in place. For example, some nuclear processes require glovebox work in close proximity to radioactive and mechanical hazards. Working in glovebox gloves can limit dexterity and increase the chance for an ergonomic injury due to constrained and/or repetitive movement. It may be possible to eliminate most hazards with the use of robotic manipulators. For this reason, the laboratory is working with the Nuclear Robotics Group at the University of Texas at Austin to develop industrial robotic manipulator controls to perform some TA-55 Plutonium Facility (PF-4) tasks which are currently completed manually by radiation workers. There are a wide variety of applications where robotic manipulation could be implemented at PF-4. These applications can be split into two broad task categories: contact and non-contact tasks. The first category includes tasks where the robot needs to make contact with the environment, such as assembly, disassembly, or packaging. Non-contact tasks include radiological surveys, storage inventory, and inventory visual inspection. This poster presents work being done in both categories which could have applications in a large number of processes at PF-4. When working on non-contact tasks, it is often difficult to ensure predictable movement of a robotic manipulator in an unknown environment. Toward this end, a Descartes path planner application is being developed for smooth motion with minimized joint reconfigurations. Contact task controllers are often built for very specific applications and are not always easily extended to multiple tasks. To make the use of robotics for contact tasks at PF-4 more feasible, a general contact task controller that can be configured for many simple contact tasks is also being developed.

**Name:** Christopher White

**Program:** GRA

**School:** New Mexico Tech

**Group:** IPM

**Mentor:** Eglin, Judith Lynne

**Category:** Engineering

**Type:** Group Poster

**LA-UR:**

# Fire Suppression System Testing Within a Closed Glovebox

Various dry chemical fire suppression systems are being considered for installation in gloveboxes. They are typically engineered systems with requirements based on the volume of the enclosure, combustible material, air flow rate, etc. Fire tests will be performed to evaluate tar the efficacy of selected fire suppression systems. The maximum airflow rate and minimum allowable working pressures for a working glovebox will be utilized as bounding criteria for fire tests to yield the most conservative and comprehensive fire test plan to suit Los Alamos National Labs (LANL) requirements.

**Name:** Micaela Christensen

**Program:** UGS/Postbacc

**School:** Taylor University

**Group:** OSH-OM

**Mentor:** Land, Whitney Morgan

**Category:** Health & Safety

**Type:** Individual Poster

**LA-UR:** 15-25492

# Ergonomic Evaluation of Anti-C Glove Transportation

In 2012, push, pull, and lift injuries cost United States businesses $15.1 billion. Los Alamos National Laboratory has reported 108 cases of such injuries in the last five years, accounting for 18.3% of all laboratory injuries. An ergonomic analysis was performed on the process of transporting Anti-C gloves into the Plutonium Facility (PF-4) at Technical Area 55. The analysis determined that many steps pose a risk for push/pull/lift injuries. Anti-C gloves are worn as an inner layer of radiation protection, in case the glovebox glove is breached. Approximately 2,400 pairs (600lbs) of Anti-C gloves are transported into the plant weekly creating many ergonomic concerns. Each bag of gloves weighs 30 lbs, and nine bags fit in every cart load. The delivery process takes two hours, and requires pushing a 300-pound cart which must be unloaded and reloaded twice per delivery. The National Institute of Occupational Safety and Health (NIOSH) Equation was used to assess the injury risk during the lifting tasks. The Lifting Index (LI) was greater than 1 which puts the worker at risk for an injury; therefore process and/or engineering solutions are needed. Two solutions will be implemented: first, installing a load dependent cart with a deck that adjusts to waist height; second, the storage cabinets will be moved outside the PF-4 turnstiles to reduce the distance traveled and the number of lifts per trip. Anthropometric data was used to determine proper shelf heights for lifting, and further calculation using the NIOSH Equation ensured the lifts were safe and had a LI of less than 1. Implementing the proposed cart and storage solutions will improve efficiency and reduce the vertical lift distances, but most importantly the risk of push/pull/lift injuries involved in the process of Anti-C glove transportation will be prevented.

Name: Jadtrl Heard

Program: GRA

School: Colorado State University

Group: NEN-2

Mentor: Mclean, Thomas Donaldson

Category: Health & Safety

Type: Individual Poster

LA-UR: LA-UR-15-25675

# Development of A Prompt Radon Detector

Exit monitors such as Hand and Foot Monitors and Personnel Contamination Monitors often alarm due to Radon daughter activity when a worker is attempting to exit a (boundary) radiologically controlled area. These alarms are a nuisance that cause time pressure, user frustration, and hinder the user's work schedule. To eliminate this issue there is a need for an instrument that can quickly and accurately differentiate radon progeny from transuranic alpha activity on personnel and clothing. An instrument based on a Xenon gas proportional probe coupled to a compact analyzer module has been developed for this specific purpose. The analyzer module enables spectroscopic and timing (i.e. pseudo-coincidence) information that be displayed on a PC or laptop to help determine the cause of the alarm. This data is displayed using a custom program written using the Python code. Data has been collected for several TRU sources as well as for Rn progeny through the use of a pylon generator. The Xe probe has also been modelled using MCNP to optimize the design for alpha detection. The goal is to develop a quick, reliable and accurate algorithm that takes account of all the data to come to a rapid decision on the nature of the activity.

**Name:** John Henry

**Program:** GRA

**School:** University of Oklahoma Health Sciences Center

**Group:** OSH-ISH

**Mentor:** Creek, Kathy

**Category:** Health & Safety

**Type:** Group Poster

**LA-UR:** LA-UR-15-25457

# Redefining Enrollment Criteria into a Hearing Conservation Program

The aim of this study is to evaluate noise exposure for MSS craft workers and define criteria for more efficient enrollment into a hearing conservation program (HCP). Workers exposed to 8 hour time weighted average noise levels over 85 decibels (dBA) require enrollment into an HCP. Currently, there is not sufficient data analysis which allows the occupational medicine professionals to confidently place or displace people into the HCP. Los Alamos National Laboratory has a responsibility to embody stewardship. Defining a more accurate and logical approach to HCP enrollment will further this principle. The data analysis examined craft worker noise levels based on a multitude of factors which include personal, area, and task oriented noise samples. The personal and task oriented noise samples provide a representative personal samples for homogenous work groups and the area samples provide a map of potential hot spots that can be considered in HCP enrollment. This study analyzed 2,266 total noise samples, 191 personal and 2075 area noise samples. Three out of the ten craft worker categories have an average exposure exceeding 85 dBA. Confidence interval interpretations suggest as many as 8 occupations could have an average exposure exceeding the threshold. With craft workers working jobs across the entire lab, area noise must be accounted for. In addition, the LANL work planning power tool database shows multiple tools recording noise readings over 100 dBA. These values approach the range of workers needing double hearing protection. Average noise exposure for craft workers exceeds the limit of 85 dBA, the primary consideration for inclusion into an HCP. With the occupation average exposure exceeding 85 dBA, work locations, and tools used on the job, craft workers qualify for enrollment into the HCP without needing prior testing. Representative personal samples for homogenous work groups and area samples should provide enough evidence for proper enrollment into a HCP.

**Name:** Anthony Van

**Program:** GRA

**School:** University of Oklahoma Health Sciences Center

**Group:** OSH-ISH

**Mentor:** Creek, Kathy

**Category:** Health & Safety

**Type:** Group Poster

**LA-UR:** 15-25457

# Redefining Enrollment Criteria into a Hearing Conservation Program

The aim of this study is to evaluate noise exposure for MSS craft workers and define criteria for more efficient enrollment into a hearing conservation program (HCP). Workers exposed to 8 hour time weighted average noise levels over 85 decibels (dBA) require enrollment into an HCP. Currently, there is not sufficient data analysis which allows the occupational medicine professionals to confidently place or displace people into the HCP. Los Alamos National Laboratory has a responsibility to embody stewardship. Defining a more accurate and logical approach to HCP enrollment will further this principle. The data analysis examined craft worker noise levels based on a multitude of factors which include personal, area, and task oriented noise samples. The personal and task oriented noise samples provide a representative personal samples for homogenous work groups and the area samples provide a map of potential hot spots that can be considered in HCP enrollment. Three out of the ten craft worker categories have an average exposure exceeding 85 dBA. Confidence interval interpretations suggest as many as 8 occupations could have an average exposure exceeding the threshold. With craft workers working jobs across the entire lab, area noise must be accounted for. In addition, the LANL work planning power tool database shows multiple tools recording noise readings over 100 dBA. These values approach the range of workers needing double hearing protection. Average noise exposure for craft workers exceeds the limit of 85 dBA, the primary consideration for inclusion into an HCP. With the occupation average exposure exceeding 85 dBA, work locations, and tools used on the job, craft workers qualify for enrollment into the HCP without needing prior testing. Representative personal samples for homogenous work groups and area samples should provide enough evidence for proper enrollment into a HCP.

**Name:** Janeth Quijada

**Program:** UGS/Postbacc

**School:** California State University, San Bernardino

**Group:** ISR-DO

**Mentor:** Johnson, Travis A

**Category:** Information Technology

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25582

# Effective Cyber Security Training for Role Based Access

Understanding cyber threats and developing an effective training and awareness program is paramount to the security and stability of the information system. Since technology is a constantly evolving entity, the training and awareness program must also constantly evolve. In order to secure our systems efficiently, all users must have access to effective cyber training and awareness in order to understand the threats and risks pertaining to the privileges they hold.ISR has restructured its system specific training, which aim at pinpointing cyber security awareness and training to various user account types thereby tailoring the material to these users. The restructured training plan involves developing three curriculums, a General User, Elevated User and System Administrator curriculum, which will focus on training that is specific to the user's role.Each user has a responsibility to uphold cyber security requirements and policies as best as possible. System Administrators have a greater range of responsibilities thus hold a greater level of risk over that of a General User. With more system privileges comes greater responsibility. ISR aims at developing its cyber security-training program to reflect that concept.

**Name:** Michael Salazar

**Program:** GRA

**School:** University of New Mexico

**Group:** DCS-CSS

**Mentor:** Maestas, Brian J

**Category:** Information Technology

**Type:** Individual Poster

**LA-UR:** 15-25971

# Visually Combining a Mixed-Network Environment

Visually combining a mixed network environment can be very useful in many applications. Usually in a mixed network environment, different computer peripherals are used for each network. By using special point-to-point technology we can visually combine two separate networks on a single monitor simultaneously while keeping the data completely separate. Think logical hardware combined with Crestron programming has allowed for a user to take multiple computer inputs from separate networks and then visually display them side-by-side while maintaining complete separation.

**Name:** Shanice Brown

**Program:** UGS/Postbacc

**School:** University of Kansas

**Group:** MPA-11

**Mentor:** Kreller, Cortney

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25710'

## Mixed-Potential Sensors for Vehicle Emissions Monitoring

NOx and NH3 sensing technology is being developed for application in vehicle emissions monitoring of diesel and lean-burn gasoline engines. In lean-burn engines, Selective Catalyst Reduction (SCR) utilizes NH3 to reduce NOx. The purpose of the NH3 sensor is to ensure that the NH3 is completely consumed in the NOx reduction reaction, and ensure that NH3 is not emitted from the tailpipe. Both the NOx and NH3 sensors described herein are mixed-potential sensors that measure the non-nernstian potential of a mixture of gases. The NOx sensor is composed of La0.8Sr0.2CrO3 (lanthanum strontium chromite) and Pt electrodes with a YSZ electrolyte and a protective porous ceramic overcoat. The NH3 sensor is composed of Au and Pt electrodes with a YSZ electrolyte and porous protective overcoat. The purpose of the protective overcoat is to protect the electrodes from containments such as heavy metals and water present in harsh exhaust environments. The performance of the sensors with the protective overcoats will be compared to the performance of the sensors of the same type without the overcoat. Sensing characteristics of response time, selectivity and sensitivity will be compared and discussed.

**Name:** Daniel Christe

**Program:** UGS/Postbacc

**School:** Drexel University

**Group:** MST-8

**Mentor:** Fensin, Saryu Jindal

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25316

# Validating a Cu-Pb Interatomic Potential for Atomistic Simulations of Shock Load

Prediction of damage development and failure in materials under dynamic loading represents a fundamental grand challenge ofmaterials science. In ductile metals, dynamic fracture occurs through a process of nucleation, growth, and coalescence of voids. For high purity single-phase metals, numerous investigators have observed that voids tend to heterogeneously nucleate at grain boundaries. However, most engineering materials are comprised of more than one element. Hence, it becomes necessary to understand the affect of the presence of a second or third phase on void nucleation. In this study, we chose Cu-Pb as a model system because of low solubility of Pb in Cu, which ensures that the majority of Pb will be located at grain boundaries. Prior computational work to understandvoid nucleation at Cu-Pb interfaces indicates that voids nucleate only within Pb, regardless of the orientation of the interface. It has been postulated that melting of lead under shock loading could be the prime reason for this observation. The objective of this work is to test this hypothesis by investigating if there is a solid-to-liquid phase transformation in single crystal lead (Pb) under shock loading conditions. A recently developed Cu-Pb embedded atom method (EAM) potential is used in this study. These results are compared with available experimental data and an old Cu-Pb potential. Our results show that there is a solid-to-liquid phase transformation in Pb at 50-55 GPa under compression. However, this pressure is even lower for melting under release. As a result, it is plausible that voids prefer to nucleate in Pb because it ismelted under release and as a result has negligible shear strength. In addition, these results are in agreement with reported experimental data, validating the Cu-Pb potential for further use in investigating Cu-Pb bimetal interfaces.

**Name:** Sophia Click

**Program:** UGS/Postbacc

**School:** Knox College

**Group:** MPA-CINT

**Mentor:** Hollingsworth, Jennifer Ann

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** 15-25699

# An Exploration of Parameters in Successive Ionic Layer Adsorption and Reactions

Giant Nanocrystal Quantum Dots (gNQDs) have distinct photophysical properties that make them an attractive component for a number of biological, chemical, and engineering applications. Unlike standard commercial quantum dots, gNQDs have very thick shells of a wide bandgap material around a semiconductor core. This thick shell results in extremely unique properties for gNQDs when compared to standard QDs, including increased stability and improved photophysical properties (i.e. decreased fluorescence intermittency (blinking), photobleaching, nonradiative Auger recombination, and increased quantum yields (QY) ). To date, successful thick shell growth has been accomplished by two distinct methods; flash synthesis and monolayer-by-monolayer with Successive Ionic Layer Adsorption and Reaction method (SILAR). In the former, the amount of precursor necessary for the full shell thickness are injected simultaneously at high reaction temperatures. SILAR is a slower, more successive method, where only enough material for each monolayer is injected at a time. A defining feature of the gNQDs is the large stokes shift, which drastically decreases the overlap of the absorption and emission spectra of the dots. Since shell thickness can be tuned, this shift can be controlled (i.e. kept in the visible spectrum) while still minimizing overlap and effectively eliminating self-absorption. Through combinatorial chemistry techniques, the parameters of the SILAR reactions are tuned to find optimum conditions for shell growth. Using state-of-the-art autoreactor technology allows the synthesis of multiple reactions simultaneously while reducing batch-to-batch variation in samples. By standardizing these reactions' specific parameters, such as core size and temperature, the results can be examined to better understand their role in shell growth. We have examined the effects on photostability, QY, and blinking of core sizes ranging from 2nm-5nm at a variety of shell thicknesses with the results presented here.

**Name:** Christopher Eley

**Program:** GRA

**School:** South Carolina State University

**Group:** ISR-3

**Mentor:** Ruggiero, Christy E

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** 15-25659

# Microscopic Multi-Step Pattern Spectra Analysis

A great deal of work has been done on the evaluation of images and the information that can be retrieved from images. One central concern is the ability to compare images based on the information retrieved from pattern recognition. In this poster, we discuss effectiveness of multi-step pattern spectra similarity of images. SEM images chosen each have a singular variant to allow for more focused comparative analysis across a singular variable. The different characteristics compared include image contrast, brightness, voltage, spot change/size, optimized voltage, and optimized spot change. The given images variations pattern spectra are computed automatically and compared against back scattered and secondary electron detector system. Images are tested using a 20 step, 30 step, and 60 step pattern spectra analysis. Preliminary test show similarity and ability to compare images by these variables.

**Name:** Purnima Ghale

**Program:** GRA

**School:** University of Illinois, Urbana-Champaign

**Group:** CCS-7

**Mentor:** Junghans, Christoph

**Category:** Materials Science

**Type:** Group Poster

**LA-UR:** LA-UR-15-25700

# Task-Based Computation of the Density Matrix in QMD Using Graph Partitioning

Quantum-based molecular dynamics (QMD) simulations are highly accurate compared to MD simulations that use classical force field models, but are significantly more expensive primarily due to the calculation of the ground-state electronic density matrix P. Traditionally, P is obtained through O(N^3) diagonalization of the Hamiltonian matrix H, limiting the number of simulated atoms N to ~1000. Second-order spectral projection (SP2) is an efficient, O (N) method to obtain P for non-metallic systems, replacing diagonalization with a polynomial expansion of H that requires only matrix-matrix multiplication and addition operations. In this interdisciplinary work, we investigate graph-partitioning techniques to divide H into smaller independent sub-matrices that correspond to strong localized chemical interactions based on an undirected graph representation of P from the preceding MD time step. This allows us to divide the SP2 computation into independent sub-problems obtained from graph partitions that can be solved with a data parallel approach. To this end, we extend usual edge-cut minimization partitioning schemes that account for inter-partition interactions to reduce the size of partitions with respect to both the number of vertices per partition as well as the number of neighbor vertices in adjacent partitions. Undesirable load imbalances arise in standard MPI/OpenMP-based implementations as the partitions are generally not of equal size. Asynchronous task-based programming models mitigate load-balancing problems by efficiently scheduling parallel computations at runtime. Intel Concurrent Collections and Charm++ implementations of our graph-partitioned parallel approach to SP2 are developed and integrated into an existing QMD code. Our approach is applied to QMD simulations of representative biological protein systems with more than 10,000 atoms, exceeding size limitations of diagonalization by more than an order of magnitude.

**Name:** Sawyer Gill

**Program:** UGS/Postbacc

**School:** New Mexico Institute of Mining and Technology

**Group:** MST-6

**Mentor:** Lienert, Thomas J

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** 15-25593

# Mesoscale Dynamics and Thermal Modeling of Direct Metal Deposition

Laser additive manufacturing is a technique that produces 3-D structures by melting and deposition of metal powder using a CAD program. Samples from a single pass width, multi-step build using 304L stainless steel were prepared using standard metallographic methods and electro-etched using 10% Oxalic acid-90 % water solution at 6 volts for ~15 second. Melt pool dimensions were measured from optical micrographs using J-Mat Pro image analysis software. Results indicate that the melt pool height and width increase in a transient region over the first 5 to 7 layers of the build, and then remain constant. These results are consistent with a thermal transient period at the start of the build where considerable heat is lost to the room temperature substrate. After several layers are deposited, the pre-heat from these layers limits heat loss to the substrate, and a greater percentage of laser energy is used to melt the incoming powder thereby causing larger melt pool dimensions. These results are also consistent with results of process modeling.

**Name:** Georg Hahn

**Program:** GRA

**School:** Imperial College London, United Kingdom

**Group:** CCS-7

**Mentor:** Junghans, Christoph

**Category:** Materials Science

**Type:** Group Poster

**LA-UR:** 15-25700

# Task-Based Computation of the Density Matrix in QMD Using Graph Partitioning

Quantum-based molecular dynamics (QMD) simulations are highly accurate compared to MD simulations that use classical force field models, but are significantly more expensive primarily due to the calculation of the ground-state electronic density matrix P. Traditionally, P is obtained through O(N^3) diagonalization of the Hamiltonian matrix H, limiting the number of simulated atoms N to ~1000. Second-order spectral projection (SP2) is an efficient, O(N) method to obtain P for non-metallic systems, replacing diagonalization with a polynomial expansion of H that requires only matrix-matrix multiplication and addition operations. In this interdisciplinary work, we investigate graph-partitioning techniques to divide H into smaller independent sub-matrices that correspond to strong localized chemical interactions based on an undirected graph representation of P from the preceding MD time step. This allows us to divide the SP2 computation into independent sub-problems obtained from graph partitions that can be solved with a data parallel approach. To this end, we extend usual edge-cut minimization partitioning schemes that account for inter-partition interactions to reduce the size of partitions with respect to both the number of vertices per partition as well as the number of neighbor vertices in adjacent partitions. Undesirable load imbalances arise in standard MPI/OpenMP-based implementations as the partitions are generally not of equal size. Asynchronous task-based programming models mitigate load-balancing problems by efficiently scheduling parallel computations at runtime. Intel Concurrent Collections and Charm++ implementations of our graph-partitioned parallel approach to SP2 are developed and integrated into an existing QMD code. Our approach is applied to QMD simulations of representative biological protein systems with more than 10,000 atoms, exceeding size limitations of diagonalization by more than an order of magnitude.

**Name:** Matthew Herman

**Program:** GRA

**School:** University of Oregon

**Group:** MST-7

**Mentor:** Blair, Michael W

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** 15-25648

# Two Dimensional Correlation Spectroscopic Analysis of Irradiated Parylene C

Parylene (poly-p-xylylene), and its family of halogenated variants, have a long history for application as protective coatings and dielectric barriers. Among them, Parylene C is the most popular due to its high impermeability to moisture and corrosive environments, and its vapor deposition polymerization application which is self-initiated and un-terminated leaving an extremely pure polymer coating. In this work Fourier transform infrared (FTIR) and two dimensional correlation (2D-COS) spectroscopies were used to follow the structural alteration occurring upon X-ray irradiation of a 25µm freestanding film of Parylene C. Samples were exposed to X-ray doses up to 100,000 Gy in air atmosphere, and IR spectra were measure after each 500Gy dose application. With the help of high resolution and high sensitivity 2D-COS it was possible to gain insight into the different effects, types and mechanisms of reactions accompanying X-ray radiation of Parylene C. Two different effects of X-ray irradiation where observed. Oxidation was observed by the production of a new species absorbing in the IR at 1698 and 1744 cm-1. An increase in local ordering was observed due to the addition of oxygen into the polymer structure after X-ray irradiation by the progressive development of new bands at 1266 and 1288 cm-1. The present work is confirmation that Parylene C does experience changes from x-ray dose.

**Name:** **Nicholas Howell**

**Program:** **GRA**

**School:** **University of Oregon**

**Group:** **CCS-2**

**Mentor:** **Nadiga, Balu**

**Category:** **Materials Science**

**Type:** **Individual Poster**

**LA-UR:** **LA-UR-15-25566**

# Limit 1-Motives are Algebraic

Abstract: If X → Δ* is a smooth projective family over the punctured disk, Schmid and Steenbrink give constructions of the limit Hodge structure Hn(ψ) of the corresponding polarized variations of Hodge structure. We construct a complex of Deligne 1-motives from the log structure of the degeneration which computes the 1-Hodge substructures of Hn(ψ).

**Name:** Matthew Kroonblawd

**Program:** GRA

**School:** University of Missouri - Columbia

**Group:** CCS-7

**Mentor:** Junghans, Christoph

**Category:** Materials Science

**Type:** Group Poster

**LA-UR:** LA-UR-15-25700

# Task-Based Computation of the Density Matrix in QMD Using Graph Partitioning

Quantum-based molecular dynamics (QMD) simulations are highly accurate compared to MD simulations that use classical force field models, but are significantly more expensive primarily due to the calculation of the ground-state electronic density matrix P. Traditionally, P is obtained through O(N^3) diagonalization of the Hamiltonian matrix H, limiting the number of simulated atoms N to ~1000. Second-order spectral projection (SP2) is an efficient, O(N) method to obtain P for non-metallic systems, replacing diagonalization with a polynomial expansion of H that requires only matrix-matrix multiplication and addition operations. In this interdisciplinary work, we investigate graph-partitioning techniques to divide H into smaller independent sub-matrices that correspond to strong localized chemical interactions based on an undirected graph representation of P from the preceding MD time step. This allows us to divide the SP2 computation into independent sub-problems obtained from graph partitions that can be solved with a data parallel approach. To this end, we extend usual edge-cut minimization partitioning schemes that account for inter-partition interactions to reduce the size of partitions with respect to both the number of vertices per partition as well as the number of neighbor vertices in adjacent partitions. Undesirable load imbalances arise in standard MPI/OpenMP-based implementations as the partitions are generally not of equal size. Asynchronous task-based programming models mitigate load-balancing problems by efficiently scheduling parallel computations at runtime. Intel Concurrent Collections and Charm++ implementations of our graph-partitioned parallel approach to SP2 are developed and integrated into an existing QMD code. Our approach is applied to QMD simulations of representative biological protein systems with more than 10,000 atoms, exceeding size limitations of diagonalization by more than an order of magnitude.

**Name:** Sergio Pino Gallardo

**Program:** GRA

**School:** University of Delaware

**Group:** CCS-7

**Mentor:** Junghans, Christoph

**Category:** Materials Science

**Type:** Group Poster

**LA-UR:** LA-UR-15-25700

# Task-Based Computation of the Density Matrix in QMD Using Graph Partitioning

Quantum-based molecular dynamics (QMD) simulations are highly accurate compared to MD simulations that use classical force field models, but are significantly more expensive primarily due to the calculation of the ground-state electronic density matrix P. Traditionally, P is obtained through O(N^3) diagonalization of the Hamiltonian matrix H, limiting the number of simulated atoms N to ~1000. Second-order spectral projection (SP2) is an efficient, O (N) method to obtain P for non-metallic systems, replacing diagonalization with a polynomial expansion of H that requires only matrix-matrix multiplication and addition operations. In this interdisciplinary work, we investigate graph-partitioning techniques to divide H into smaller independent sub-matrices that correspond to strong localized chemical interactions based on an undirected graph representation of P from the preceding MD time step. This allows us to divide the SP2 computation into independent sub-problems obtained from graph partitions that can be solved with a data parallel approach. To this end, we extend usual edge-cut minimization partitioning schemes that account for inter-partition interactions to reduce the size of partitions with respect to both the number of vertices per partition as well as the number of neighbor vertices in adjacent partitions. Undesirable load imbalances arise in standard MPI/OpenMP-based implementations as the partitions are generally not of equal size. Asynchronous task-based programming models mitigate load-balancing problems by efficiently scheduling parallel computations at runtime. Intel Concurrent Collections and Charm++ implementations of our graph-partitioned parallel approach to SP2 are developed and integrated into an existing QMD code. Our approach is applied to QMD simulations of representative biological protein systems with more than 10,000 atoms, exceeding size limitations of diagonalization by more than an order of magnitude.

**Name:** Vivek Sardeshmukh

**Program:** GRA

**School:** University of Iowa

**Group:** CCS-7

**Mentor:** Junghans, Christoph

**Category:** Materials Science

**Type:** Group Poster

**LA-UR:** 15-25700

# Task-Based Computation of the Density Matrix in QMD Using Graph Partitioning

Quantum-based molecular dynamics (QMD) simulations are highly accurate compared to MD simulations that use classical force field models, but are significantly more expensive primarily due to the calculation of the ground-state electronic density matrix P. Traditionally, P is obtained through O(N^3) diagonalization of the Hamiltonian matrix H, limiting the number of simulated atoms N to ~1000. Second-order spectral projection (SP2) is an efficient, O(N) method to obtain P for non-metallic systems, replacing diagonalization with a polynomial expansion of H that requires only matrix-matrix multiplication and addition operations. In this interdisciplinary work, we investigate graph-partitioning techniques to divide H into smaller independent sub-matrices that correspond to strong localized chemical interactions based on an undirected graph representation of P from the preceding MD time step. This allows us to divide the SP2 computation into independent sub-problems obtained from graph partitions that can be solved with a data parallel approach. To this end, we extend usual edge-cut minimization partitioning schemes that account for inter-partition interactions to reduce the size of partitions with respect to both the number of vertices per partition as well as the number of neighbor vertices in adjacent partitions. Undesirable load imbalances arise in standard MPI/OpenMP-based implementations as the partitions are generally not of equal size. Asynchronous task-based programming models mitigate load-balancing problems by efficiently scheduling parallel computations at runtime. Intel Concurrent Collections and Charm++ implementations of our graph-partitioned parallel approach to SP2 are developed and integrated into an existing QMD code. Our approach is applied to QMD simulations of representative biological protein systems with more than 10,000 atoms, exceeding size limitations of diagonalization by more than an order of magnitude.

**Name:** Benjamin Schilling

**Program:** UGS/Postbacc

**School:** New Mexico Tech

**Group:** M-9

**Mentor:** Dattelbaum, Dana Mcgraw

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25410

# Shock Characteristics of UHMWPE and HDPE

High-density polyethylene (HDPE) and ultra-high-molecular-weight polyethylene (UHMWPE) are widely used thermoplastics in several industries for a multitude of applications. In this study, the dynamic response of HDPE and UHMWPE was determined for a pressure range from 0.32-19.58 GPa in an effort to further understand their behavior under dynamic high pressures and to validate Mori's results that polyethylene (PE) exhibits a nonlinear Hugoniot curve at particle velocities of ~150 m/s [1]. The wave profiles for the HDPE data shows that there is multi-wave structure when the particle velocity is around 160 m/s, which is indicative of a phase change happening in the material. The HDPE data obtained from Los Alamos National Laboratory matches some of the points on Mori's Us-Up graph, but from the data obtained thus far, there is no real indication of a nonlinear Hugoniot for HDPE. On the other hand, the data obtained for UHMWPE lines up well with Mori's data, which could be an indication that the Hugoniot is nonlinear at low particle velocities for UHMWPE.

**Name:** Jerry Shi

**Program:** GRA

**School:** The University of Georgia

**Group:** CCS-7

**Mentor:** Junghans, Christoph

**Category:** Materials Science

**Type:** Group Poster

**LA-UR:** LA-UR-15-25700

# Task-Based Computation of the Density Matrix in QMD Using Graph Partitioning

Quantum-based molecular dynamics (QMD) simulations are highly accurate compared to MD simulations that use classical force field models, but are significantly more expensive primarily due to the calculation of the ground-state electronic density matrix P. Traditionally, P is obtained through O(N^3) diagonalization of the Hamiltonian matrix H, limiting the number of simulated atoms N to ~1000. Second-order spectral projection (SP2) is an efficient, O(N) method to obtain P for non-metallic systems, replacing diagonalization with a polynomial expansion of H that requires only matrix-matrix multiplication and addition operations. In this interdisciplinary work, we investigate graph-partitioning techniques to divide H into smaller independent sub-matrices that correspond to strong localized chemical interactions based on an undirected graph representation of P from the preceding MD time step. This allows us to divide the SP2 computation into independent sub-problems obtained from graph partitions that can be solved with a data parallel approach. To this end, we extend usual edge-cut minimization partitioning schemes that account for inter-partition interactions to reduce the size of partitions with respect to both the number of vertices per partition as well as the number of neighbor vertices in adjacent partitions. Undesirable load imbalances arise in standard MPI/OpenMP-based implementations as the partitions are generally not of equal size. Asynchronous task-based programming models mitigate load-balancing problems by efficiently scheduling parallel computations at runtime. Intel Concurrent Collections and Charm++ implementations of our graph-partitioned parallel approach to SP2 are developed and integrated into an existing QMD code. Our approach is applied to QMD simulations of representative biological protein systems with more than 10,000 atoms, exceeding size limitations of diagonalization by more than an order of magnitude.

**Name:** Orion Staples

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** EES-17

**Mentor:** Saleh, Tarik A

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25391

# Nonlinear Elasticity Analysis of Deformed vs. Non-deformed Metals

Through the use of Resonant Ultrasound Spectroscopy (RUS), and Nonlinear RUS, the linear and nonlinear elastic properties of a material can be determined by analyzing the different resonance frequencies. These experimental resonance frequencies are then compared against the predicted frequencies (determined through the use of modeling) in order to determine the linear elastic properties, Young's Modulus and Poisson's Ratio, and nonlinear property, alpha. This research focused on experimentally determining the elastic properties of tantalum as it has a density near that of plutonium. After this material was analyzed and characterized, it was deformed by a high strain rate Taylor Anvil experiment. Following the experimental characterization, Nonlinear Resonant Ultrasound Spectroscopy (NRUS) was performed in order to determine the presence of internal nonlinearities, e.g. micro cracks. This technique involves analysis of the lowest resonance frequency, and examines how the elastic properties change as the strain amplitude is increased. This research was performed on tantalum to ensure accuracy of these methods when utilized on plutonium tensile samples.

**Name:** Andrew Stine

**Program:** GRA

**School:** University of Dayton

**Group:** MET-1

**Mentor:** Pierce, Stanley W

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25498

# Evaluation of Molybdenum as a Surrogate for Iridium in the GPHS Weld Development

A General Purpose Heat Source (GPHS) is used to provide power for spacecraft. The GPHS consists of a Pu-238 pellet encased within a Gas Tungsten Arc (GTA) welded iridium clad. The current welding system is twenty five years old and is undergoing an upgrade. The welding procedure has also remained unchanged since installation, and this will also be looked at for potential improvement. Weld development and qualification requires numerous test welds and material samples, but this effort is severely limited due to the high cost of iridium components. A less expensive metal with similar welding characteristics could provide the opportunity to more fully investigate and test the weld process prior to qualification using iridium. One such metal is molybdenum since its melting index (melting temperature x thermal conductivity) is closest to iridium. This means that welds on molybdenum and iridium should be similar in size and grain structure; both main factors in weld strength and quality. The 2" diameter iridium blank disc that the clad cup is formed from is good for initial weld trials and cost $5000 each, versus a development clad set that cost $15,000. Meanwhile a single molybdenum disc costs only $9. To evaluate molybdenum as a surrogate for iridium, GTA welds were developed to provide full penetration on molybdenum discs at speeds of 20, 25, and 30 inches per minute (ipm) and then these weld parameters were repeated on iridium. The top surface (overbead), bottom surface (underbead), and grain structure of the molybdenum and iridium welds were compared. It was found that weld conditions transferred well from molybdenum to iridium, producing similar weld widths and similar tendencies in solidification structure. Molybdenum discs and tube sections will greatly expand the weld testing opportunities prior to iridium weld qualification.

**Name:** Katey Thomas

**Program:** UGS/Postbacc

**School:** New Mexico Institute of Mining and Technology

**Group:** M-9

**Mentor:** Gustavsen, Rick

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25403

# Experimental Studies of Rod-Impact on Composition B-3

The initiation of detonation in an explosive due to fragment impact has been studied a lot in the past several decades. Most work focused on finding the velocity at which an explosive has a 50% probability of detonating. More recent research is focusing on the mechanism that leads to the detonation: classical shock to detonation transition or shear driven ignition. In a series of rod-impact experiments at ~745 m/s by Gustaven, et al. (2013) on PBX 9501 and modeled by hydrodynamic codes, shear was not the dominant factor in initiation. In the present series of rod-impact experiments, we used a 12.5-mm diameter, 304L stainless steel rod to impact Composition B-3 at ~100 m/s and recorded the result using a high-speed video camera. (Composition B-3 is a 60/40 mix of RDX and TNT. It has approximately the same shock sensitivity as PBX 9501, but is much more brittle.) In our experiments, we kept the rod diameter and velocity constant and varied the sample thickness, whether or not there was a PMMA window on the back of the sample, and finally the temperature of the sample. The first experiments show Comp-B deflagrating as a result of shear displacement. Further experiments will investigate whether the deflagration transitions to detonation.

**Name:** Matthew Ticknor

**Program:** UGS/Postbacc

**School:** University of Utah

**Group:** MPA-CINT

**Mentor:** Hollingsworth, Jennifer Ann

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25708

# Creating Metal or Nanoparticle Arrays Using Langmuir-Blodgett Methodologies

The technique of nanosphere lithography was used to create well-ordered arrays of metal islands. This entails first depositing onto silicon substrate hexagonal arrays of polystyrene (PS) microspheres (495 nm diameter) by self-assembled Langmuir-Blodgett deposition. The PS sphere layer can then used as an ‘evaporation mask’. The Langmuir-Blodgett (LB) technique of shadow nanosphere lithography was investigated and used to consistently create series of well-ordered arrays. The consistency which can be achieved using an LB system is what made it an ideal method of deposition. The clean substrate was coated with the polystyrene beads through vertical LB deposition. In order to find an ideal angle, which is less than ten degrees, the angle of solutions was measured using a contact angle meter. It was important to characterize the contact angle of the bead solutions on the silicon substrate. This was done in order to help determine a cleaning method, and to understand the likelihood of bead deposition. Once an ordered array has been deposited, the substrate then undergoes an HF treatment, which allows for a smoother deposition of a thin film of metal. After metal deposition the can be used as catalysts for solution-phase semiconductor nanowire growth. The resulting ordered nanowire arrays can be used in solar energy harvesting and next generation lighting. Alternatively, the metal arrays may also studied for new magnetic behavior which may be created as a result of interactions between the individual islands

**Name:** Phillip Weiner

**Program:** GRA

**School:** University of Southern California

**Group:** MPA-CINT

**Mentor:** Hollingsworth, Jennifer Ann

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25667

# Near-Unity Down-Conversion Efficiency in Giant Quantum Dot Light-Emitting Diodes

Poster presenter: Phil Weiner Poster contributors: Christina J. Hanson, Han Htoon, Jennifer A. Hollingsworth Specific shades of white-light can be created by using emissive color-converting materials in conjunction with primary colored light emitting diodes (LEDs). The current industry standard uses a broadband yellow phosphor (cerium(III) doped yttrium aluminum garnet, or YAG:Ce3+) to down-convert light from a blue LED, which has an expansive emission range but a high level of stability and efficiency. The next generation of commercial solid-state lighting demands higher quality white-light, requiring the development of a new red-emitting down-conversion phosphor with narrowband emission. Semiconductor quantum dots (QDs) have long been investigated for this purpose due to their tunable and specific emission range, and possible 100% quantum yield in solution, but these lack practicality due to issues with photostability and self-reabsorption in the solid state. A new class of QD with a thick inorganic shell, called “giant” quantum dots (gQDs), has been shown to circumvent many of these issues, and here are investigated as down-conversion phosphors in the form of a solid polymer composite. The gQD composites were investigated for their down-conversion efficiency and relative photoluminescence (PL) intensity while exposed to (1) temperatures ranging from 25° to 95° C and (2) variable levels of photon flux (achieved by varying LED driving current). A polymer matrix composition was chosen that allowed for virtual equivalency between the solution and solid-state quantum yields (emission efficiencies). Additionally, incorporation of a thin ‘spacer layer’ in the devices afforded substantially reduced thermal or photon-flux quenching otherwise dominant at high driving currents (>200 mA).

**Name:** Ximone Willis

**Program:** UGS/Postbacc

**School:** University of Texas at Dallas

**Group:** MPA-CMMS

**Mentor:** Balakirev, Fedor Fedorovich

**Category:** Materials Science

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25287

# 3D Printed Cryogenic Probes for High Magnetic Fields

The materials used in constructing probes for high magnetic fields have a very specific set of requirements: they must be cold-tolerant, non-ferrous, and durable. Tiny measurement volume available at highest magnetic fields requires high manufacturing precision. With the recent advances in plastics,3D printing is fast becoming a viable technology for manufacturing probes. We designed and tested sample rotator probe to be used in 100 Tesla pulsed magnet. Several functional probe prototypes were constructed via a number of different additive manufacturing techniques to identify materials and methods suitable for cryogenic applications in high magnetic fields.

**Name:** William Casper

**Program:** GRA

**School:** University of Washington, Seattle

**Group:** CCS-2

**Mentor:** Nadiga, Balu

**Category:** Mathematics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25567

# Elementary Solutions to Bochners Problem for Matrix Differential Operators

We demonstrate an elementary method for constructing new solutions to Bochner's problem for matrix differential operators from known solutions. We then describe a large family of solutions to Bochner's problem, obtained from classical solutions, which subsume several examples known from the literature. Then by virtue of the method of construction, we show how one may explicitly identify a generating function for the associated sequences of monic orthogonal matrix polynomials as well as the associated algebra of idfferential operators for which the polynomials are eigenfunctions.

**Name:** Jennifer Lilieholm

**Program:** GRA

**School:** University of Washington

**Group:** XTD-NTA

**Mentor:** Ramsey, Scott D

**Category:** Mathematics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25347

## Lagrangian Hydrocode Initialization Methods for the Converging/Diverging Shock

The Guderley Problem models a strong converging spherical shock that reaches the origin with infinite pressure, which generates an outgoing shockwave. Though the Guderley Problem is simple to grasp conceptually, it is difficult to simulate in a hydrocode because it lacks an analytic solution describing the two shocked regions. However, Lie group analyses of the Euler compressible flow equations resulted in a set of ordinary differential equations describing the shock. These can be solved through the use of a mathematical software package, such as Mathematica. This solution takes the form of an interpolating function, which can then be input as a set of field variables into code for initialization of the Guderley Problem (direct method). An alternative method of initialization is to find the equation of motion for a piston that moves into the unshocked region, generating the desired shock ahead of itself (piston method). Both initialization methods were used to initialize the Guderley Problem in FLAG (a LANL hydrocode), and a quantitative code verification analysis was performed to determine the comparative accuracy of the two strategies. The piston initialization method had lower unweighted L1 error norms than the direct method, but the volume and mass weighted error norms were smaller for the direct method than the piston. This is due to the majority of the piston error being located at a large radius, near the outer boundary that behaves as a piston, which is known as a wall-heating error. The direct method, on the other hand, was accurate at a distance, but had greater error near the shock wave than the piston did. Despite the differences in accuracy, both methods were found to be first order convergent in space, as expected for shock simulations, and appear to be valid strategies for initializing the Guderley Problem in FLAG.

**Name:** Heather Hughes

**Program:** GRA

**School:** Arizona State University

**Group:** CPA-CAS

**Mentor:** Basquin, Susan C

**Category:** Non-Technical

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25389

## Learning English as an Adult: Sociolinguistics and Second Language Acquisition

This secondary research project explores the research and literature addressing adult English Language Learners (ELLs) in relation to idioms. Specifically, it examines the importance of teaching American idioms in the English as a Second Language (ESL) classroom and how not including American idioms in classroom practices can negatively impact the adult ESL students' second language acquisition. It also examines current teaching practices and how they could be used to guide adult ESL students' through learning American idioms. The secondary research project proposes that, based on the investigation that there is a need to systematically incorporate the teaching of idioms into the adult second language (L2) curricula. To that end, adding an idiom-specific course to the adult L2 curricula at the university level will close the language gap between formal classroom language and real life language.

**Name:** Blake Benyard

**Program:** UGS/Postbacc

**School:** Morehouse College

**Group:** NEN-3

**Mentor:** Winkler, Ryan

**Category:** Other

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25585

# Characterization of Handheld Detectors for Nuclear Detection and Identification

The performance of two commonly used instruments, the FLIR systems IdentiFINDER and identiFINDER2 are characterized in this work. These devices each contain a Sodium Iodide (NaI) crystal, the most popular scintillation material for the detection of gamma ray emission. Performance characteristics such as full width at half maximum (FWHM), detector gain, and linearity of the two detectors are investigated as a function of count rate. Measurements consisted of the detection of gamma ray emission from a series of sources, Na-22, Co-60, and Np-237, placed at a variety of source-detector distances. Spectrum data and isotopic identifications were saved on each device and exported to the spectrum analysis software PeakEasy, where photopeak centroids and FWHM were determined. Spectra were individually re-calibrated to investigate the linearity of the detectors as a function of count rate using the R programming language. The detector gain and FWHM remained constant for the count rates but there is a significant difference in the linearity of the two detectors. These results show that while the linearity of both detectors doesn't change with count rate, the identiFinder2 displays significant non-linear behavior compared to the identiFINDER.

**Name:** Kenneth Gibson

**Program:** GRA

**School:** Alcorn State

**Group:** NEN-3

**Mentor:** Simpson, Ches

**Category:** Other

**Type:** Individual Poster

**LA-UR:** 15-25584

# Using R to Analyze Detector Data

Efficiency and other measurements of several High Purity Germanium (HPGe) detectors were taken using up to three radioactive sources (Eu-152, Th-228 and a 10 isotope cocktail). The resulting data was then manipulated using the R, programming language, a free software primarily used in statistical research and data analysis. Herein R has been applied to the analysis and display of full-width-at-half-maximum (FWHM), efficiency, and virtual point (aka effective center) data of several HPGe detectors. Within R, mathematical manipulation, error propagation, linear and nonlinear curve fitting routines were used to generate plots of efficiencies and FHWM data versus energy for EX-100 and micro detective units. Determining these detector parameters helps radiation detection scientists to determine unknown source activities and detector modeling parameters.

**Name:** Lauren Liegey

**Program:** UGS/Postbacc

**School:** Truman State University

**Group:** NEN-5

**Mentor:** Wilcox, Trevor ;

**Category:** Other

**Type:** Individual Poster

**LA-UR:** LA-UR-15-24994

# Predicting Future Solar Modulation

The annual values of the of the modulation parameter, ϕ, have been recorded since 1936, and their fluctuation is seen to be roughly sinusoidal over time. The current data available only reports solar modulation until year 2014. We sought to predict how the solar modulation of cosmic background radiation reaching the earth's surface fluctuates for dates beyond 2014. We wrote a program that uses the most recent past solar modulation data to create a sinusoidal fit curve to that data. This fit is then extrapolated to the year for which the prediction is desired, giving an estimate for the solar modulation parameter in the future. We present our method of obtaining the fit and a discussion on its accuracy and how we determined that accuracy. Also included is a description of how this program, along with others, may be implemented in MCNP to improve the code's simulation of overall background radiation.

**Name:** Alexander Ortiz

**Program:** UGS/Postbacc

**School:** Northwestern University

**Group:** XCP-6

**Mentor:** Tierney, Heidi E. Morris

**Category:** Other

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25079

# Geo-Location of Atmospheric Radio Radiation Using Ground-Reflected Signals

Abstract. Radio sources originating above the surface of the earth are not always isotropic, and, therefore, will not necessarily have a strong signal that travels via a direct path to a satellite. An example of this is an impulsive radio signal from a relativistic electron avalanche moving downward toward the earth. Its radiation lobes are strongest near the direction of propagation. It is possible that only ground-reflected signals from such sources would be received by satellite-borne sensors. Time-of-arrival algorithms based on the detection of the direct pulse would then incorrectly locate the source of the radiation. We will develop a method to locate a source of earth-directed radiation by taking into account the additional flight path of the reflected signal. We will first consider the vacuum environment and ideal reflection off the earth's surface (Snell's Law). The method will reveal how many satellite sensors are required to locate the source. We conclude by exploring a solution to the problem of geolocating a source based on time-difference-of-arrival (TDOA) data collected by an array of sensors above the surface of the earth.

**Name:** Celeste Bean

**Program:** UGS/Postbacc

**School:** University of California, Santa Barbara

**Group:** T-6

**Mentor:** Newell, Raymond Thorson

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25518

# Galois/Counter Mode Encryption for Quantum Communications in the Power Grid

The United States' "smart" electric grid uses two-way communication and information processing to generate remarkable improvements in the grid's efficiency, but substations currently transmit unencrypted and unauthenticated signals containing data about energy use, leaving critical vulnerabilities to cyberattacks. A 2015 report from the University of Cambridge's Center for Risk Management estimated that a cyberattack on the northeastern United States could leave 93 million people without power, decimate healthcare infrastructure, and cost more than $1 trillion USD in damages. Galois/Counter Mode (GCM) Encryption, using keys generated by Quantum Key Distribution (QKD), represents a quantum cryptographic scheme that ensures digital communications' encryption, authentication, and integrity while also negating crucial vulnerabilities. QKD forms a shared, secret key inherently protected from eavesdropping by potential adversaries. GCM then uses the key in authenticated encryption and decryption algorithms that are highly parallelized and thoroughly pipelined to authenticate the signal's source and confirm its integrity. Encrypting signals with a key based in quantum mechanics promises the secrecy and indistinguishability of the transmitted information. The authentication methods use a universal hash function defined over a binary Galois field to allow information to be sent in the clear while still guaranteeing the legitimacy of the data's origin—this property permits sending both unencrypted control signals and other necessarily encrypted information. Finally, GCM validates signals' integrity, ensuring that signals have not been modified either accidentally or maliciously during their transmission.

**Name:** Shane Coffing
**Program:** UGS/Postbacc
**School:** New Mexico Tech
**Group:** XCP-1
**Mentor:** Bement, Matt
**Category:** Physics
**Type:** Individual Poster
**LA-UR:** LA-UR-15-25605

# Computing the Self-Diffusion Coefficient in Warm Dense Matter

Warm dense matter (WDM) describes a temperature and density regime for matter that lies roughly between plasma and solid states. Self-diffusion refers to the thermal motion of a single particle throughout a pure or mixed substance. Aside from a fundamental theoretical interest, self-diffusion is a transport property and is useful in the simulation of WDM in inertial confinement fusion, stellar evolution models, and other hydrodynamic plasma experiments. However, the experimental determination of the self-diffusion coefficient is very difficult and indirect, and molecular dynamics simulation is most commonly used for its determination. Currently there are two widely used methods of obtaining the self-diffusion coefficient D with molecular dynamics. One is by means of solving the Green-Kubo relation, which relates the diffusion coefficient to the integration of the velocity auto-correlation function. The other method to obtain D is by solving the Einstein relation, which expresses D in terms of the mean squared displacement. However, the generation of tables of diffusion coefficients using these methods is not easily automated. A third method for obtaining D that promises easier automation is introduced here: computing D from the Gaussian approximation to the self van Hove function, which is a function that describes where a particle is at some later time relative to its starting position.

**Name:** Melissa Compton

**Program:** UGS/Postbacc

**School:** University of Missouri - Columbia

**Group:** P-25

**Mentor:** Tupa, Dale

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** 15-25523

# Building and Testing a Four Unit PDV

PDV (Photon Doppler Velocimetry) is an optical diagnostic used to determine the velocity of a moving surface by using reflected Doppler-shifted laser light. The laser light is split, where ten percent of the light is directly reflected, and ninety percent is reflected off of the moving surface, thus it is Doppler shifted. The two reflections then come back together with different frequencies, creating a beat frequency. The data collected is then analyzed using a Fourier transform, to determine the velocity of the surface. The high sensitivity of this diagnostic gives it a broad range of applications for high velocity or vibrating objects. At the Proton Radiography Facility, PDV is used in dynamic experiments where a proton beam images high explosives interacting with different materials. We constructed a four unit PDV box capable of measuring the velocity at four points on the surfaces of the materials in these experiments. In order to test the PDV, we designed and constructed a calibration box that uses a Dremel tool with a whirling circular blade. The blade spins at a known frequency, so we can predict the velocity we will measure with the PDV.

**Name:** Tess Daughton

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** P-25

**Mentor:** Bacon, Jeffrey Darnell

**Category:** Physics

**Type:** Group Poster

**LA-UR:** 15-25464

## Supplemental Measurement for a New Method of Nuclear Missile Warhead Detection

Muons are highly penetrative subatomic particles created from collisions between cosmic rays and Earth's atmosphere. Muons are an excellent tomographic tool due to the fact that muon imaging does not introduce additional radiation exposure, unlike X-ray imaging, and can be used to probe highly dense materials. Muon Tomography was developed at Los Alamos National Laboratories by Christopher Morris and William Priedhorsky in 2001 and has been further developed for a plethora of applications. One of these applications is the detection of shielded fissile material. This occurs by using a combination of muon and neutron detectors to pinpoint locations in which a low-energy muon was stopped in the material and induced fission. A limitation of this technique is the lack of data regarding the low end of the muon energy spectrum. High-energy muons will pass through the fissile material easily while low-energy muons will stop and induce a reaction. This research will measure the percentage of muons that are low-energy by using lead as an equal substitute for a fissile material such as uranium. This research will enhance the fissile material detection technique.

**Name:** Patrick Denne

**Program:** GRA

**School:** University of New Mexico

**Group:** XCP-6

**Mentor:** Bradley, Paul Andrew

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25508

## Equations of State for Nickel Aluminum in the Warm Dense Matter Regime

Dalton's Law and Amagat's Law were developed in order to describe the behaviors and properties of mixtures of ideal gases. These mixture rules are being used today to describe the equation of state of several multi-component materials. These materials are generally in the high energy density or warm dense matter regime. There exists little data about certain metal mixtures when they are at pressure of above 10 megabars. The predictions offered by Dalton's Law and Amagat's Law show increasing disagreement for NiAl mixtures that we study here. Recently fielded experiments focused on the equations of state for nickel, aluminum (Swift, Paisley, McClellan, Ackland, 2007), and a nickel/aluminum alloy. A ramp pulse from the Omega-EP laser lasting four nanoseconds provides a shock that allows us to determine the properties of these materials and their alloys, and the RAGE code is being used to model the experiments. These tools should allow us to discern whether Dalton's Law or Amagat's Law is more useful for the predictions of NiAl alloy equations of state behavior in the warm dense matter regime.

**Name:** Laura Elgin

**Program:** GRA

**School:** University of Michigan

**Group:** XTD-IDA

**Mentor:** Mussack Tamashiro, Katie

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25490

# Modeling Heat Flow for Proposed Experiments to Measure Opacities in HED Plasmas

We are developing a proposal for experiments at The National Ignition Facility (NIF) to measure opacities of elements with atomic numbers in the range of 6-10 at temperatures and densities relevant to the base of the solar convection zone, other astrophysical bodies, and applications in ICF. Our proposed experiments would provide the first opacity measurements for these elements within this high-energy-density (HED) regime. A critical feature of our experimental platform is a super-sonic radiation front propagating within the target materials. With a sufficiently supersonic radiation front, the density of the heated material (behind the front) remains constant and equal to the density of the cold material (ahead of the front) over a time scale of a couple nanoseconds. Afterwards, hydrodynamic effects create temperature and density gradients within the heated material, which would obfuscate analysis of opacity data. Therefore, there exists a brief time window during which the opacities of both the hot and cold material may be measured at constant and well-known densities. We are using xRage to simulate heat flow within our targets in order to estimate the time scale over which significant temperature and density gradients evolve. These simulations will better inform our target design and requirements for the spectral, spatial, and temporal resolution of the diagnostics to be used in the proposed experiments. If successful, our experiments could yield the data necessary to validate existing opacity models or provide physical insights to inform the development of new opacity models. Accurate opacity models are essential to the understanding of radiation transport within high-energy-density systems, with applications ranging from astrophysics to ICF.

**Name:** Ebraheem Farag

**Program:** UGS/Postbacc

**School:** The Ohio State University

**Group:** XTD-IDA

**Mentor:** Mussack Tamashiro, Katie

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25494

# Using New ATOMIC Opacities in MESA Solar Models

The study of opacities and their effect on solar models is a current area of astrophysics in need of clarification. Through mapping of resultant abundances and sound speeds of elements z1-z30 contained in many 2nd and 3rd generation stars, this project attempts to show the extent to which varying opacities can impact our current understanding of star formation and evolution. This is done using MESA stellar modeling code, and with LANL stellar pulsation codes, along with new unreleased ATOMIC opacity tables also developed at The Los Alamos National Laboratory. This project serves as one examination of how these new opacities can alter our models of the sun, and in turn their usefulness in modeling other stars, light years distant. The sun is considered mostly hydrogen, but sparse traces of other heavy elements living inside lend a hand in determining the flow of radiation and energy through the stellar interior. For this reason, the study of these elements is of great importance. These models are increasingly essential, since most observations scientists make about other stars are derived from knowledge obtained with respect to our sun. The models generated in this project are intended to help bring current sound speed models closer to inferences from modern helioseismic data. Nonetheless, other changes to the physics included in stellar models are necessary to achieve the desired levels accuracy this area of astrophysics deserves.

**Name:** George Fuller

**Program:** UGS/Postbacc

**School:** University of California Santa Barbara

**Group:** T-2

**Mentor:** Hayes-Sterbenz, Anna Catherine

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25693

# Neutrino Cross Section of Interaction With Helium-4 Nuclei

Using updated calculations of the energy eigenstates of the 4He nucleus and the no core shell model of atomic nuclei, we have produced a more accurate calculation of the cross section for interaction between neutrinos/antineutrinos and 4He for both neutral- and charged-current interactions. Previous calculations of this cross section were performed by only taking into account the strong contribution from Gamow-Teller transitions and neglecting the higher-order operators which allow transitions to other states. The Gamow-Teller-only approximation for the neutrino cross section is efficacious for the needs of most Standard Model Big Bang nucleosynthesis calculations, where the neutrino cross section of 4He is not a significant contributor to neutron and deuterium abundance. However, using the Gamow-Teller-only approximation strains the bounds on the accuracy needed by newer calculations which aim to include Beyond-Standard Model effects for reproducing precise cosmological data. By including all energy eigenstates in the calculation and including the effects from the energy widths of each state, we can provide a neutrino energy-dependent 4He cross section which meets these higher needs of precision.

**Name:** Robin Heinonen

**Program:** GRA

**School:** University of California San Diego

**Group:** XCP-5

**Mentor:** Saumon, Didier

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25546

# Coefficients of Diffusion in Dense Stellar Plasmas

The Sun and the vast majority of stars will end their lives as white dwarf stars, cooling nuclear embers that pack about half the mass of the Sun within the volume of a small planet like the Earth. As a consequence, white dwarfs present exotic physical conditions that cannot be reproduced in the lab. In particular, their high surface gravity causes the elements to sort themselves by atomic weight because heavier elements diffuse downward on relatively short time scales. In a particular class of white dwarfs, the surface layers are made of nearly pure helium with traces of heavier elements such as Si, Ca, Na, and Mg. These "polluting" elements are accreted as solid planetary material (dust or asteroids) and gradually diffuse into the star. We present a new study of the physics of diffusion in the dense plasmas found in white dwarfs stars to update a theory that is now 30 years old. Using a combination of new dense plasma models and modern computational approaches, we calculate the inter-diffusion coefficient of Ca and of Si in a dense He plasma in two different ways. Both are found to agree very well over a wide range of plasma conditions found in white dwarfs. However, we find differences with the standard values used in modeling diffusion in white dwarf stars of up to a factor of 2. We also find that, contrary to previous results, Ca diffuses more slowly than Si in white dwarfs, which has implication for the inferred composition of the accreted planetary material.

**Name:** John Jacobs

**Program:** UGS/Postbacc

**School:** University of Rochester

**Group:** XCP-6

**Mentor:** Rousculp, Chris

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25611

# Modeling High Precision Liner Implosions using Magnetohydrodynamic Codes

Liner implosions are a proposed method for generating warm dense matter (WDM). They work by pumping current through a small conductive cylindrical liner, causing it to implode onto a target at high speeds due to the Lorentz force. To achieve the extreme speeds required, tens of mega-Amps must be delivered to a cylinder of relatively small mass. Under these extreme conditions Ohmic heating causes the liner to melt. The challenge is that, to achieve uniform compression of the target as is desired, the liner must remain mostly solid, as liquids are subject to Rayleigh-Taylor (RT) instabilities. One recently proposed method to achieve this is called “Kick and Coast”. It relies on the principle that the smallest amount of melting occurs when the majority of the current pulse, and therefore acceleration, is applied in a short burst and to a large diameter liner. After this initial “kick” the cylinder “coasts” with little to no acceleration (and thus little additional Ohmic heating) until it’s diameter becomes small enough that the material’s inner surface is pushed rapidly inward by the incompressible thickening of the cylinder, providing a final boost of acceleration. To test the relative merits of this alternate approach, simulations were first run using a 1-D magnetohydrodynamics (MHD) code called RAVEN. This code, being one dimensional, has a short runtime, which allowed us to create a large, varied test base of runs. As RAVEN does not account for RT instabilities, a candidate configuration was selected from these 1-D runs (based on minimal melting and high final velocity) to be run on the more complete 2-D MHD code, FLAG. The results of this run are currently pending, but if they show that the Kick and Coast method can be used to achieve high speed, uniform liner implosions, it will provide a viable platform for generation of WDM.

**Name:** Olivia Johnson

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** P-25

**Mentor:** Bacon, Jeffrey Darnell

**Category:** Physics

**Type:** Group Poster

**LA-UR:** 15-25464

# Supplemental Measurement for a New Method of Nuclear Missile Warhead Detection

Muons are highly penetrative subatomic particles created from collisions between cosmic rays and Earth's atmosphere. Muons are an excellent tomographic tool due to the fact that muon imaging does not introduce additional radiation exposure, unlike X-ray imaging, and can be used to probe highly dense materials. Muon Tomography was developed at Los Alamos National Laboratories by Christopher Morris and William Priedhorsky in 2001 and has been further developed for a plethora of applications. One of these applications is the detection of shielded fissile material. This occurs by using a combination of muon and neutron detectors to pinpoint locations in which a low-energy muon was stopped in the material and induced fission. A limitation of this technique is the lack of data regarding the low end of the muon energy spectrum. High-energy muons will pass through the fissile material easily while low-energy muons will stop and induce a reaction. This research will measure the percentage of muons that are low-energy by using lead as an equal substitute for a fissile material such as uranium. This research will enhance the fissile material detection technique.

**Name:** David Liddle

**Program:** UGS/Postbacc

**School:** Austin Community College

**Group:** C-IIAC

**Mentor:** Engle, Jonathan Ward

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25525

# Isotope Production Target Design and Cross-Section Compilation and Analysis

The overall goal of the internship assignment was to perform research projects in accordance with the Los Alamos National Laboratory (LANL) mission statement [1]. Intern contributions include the design of a target capsule and holder for a 238U target foil to be irradiated by proton beam, and the compilation and analysis of nuclear reaction cross sections for proton-induced reactions on 232Th. The target capsule and holder designs for the Isotope Production Facility (IPF) will aid in the direct production of 236gNp, as well as the production of 236Pu via decay of 236mNp. The production of 236gNp supports the need for isotope dilution standards identified by the Nuclear Science Advisory Committee (NSAC) Isotopes Subcommittee in its "Compelling Research Opportunities Using Isotopes" report [2]. Both of the radionuclides produced will help researchers to detect and quantify 237Np and 238Pu for environmental protection, nonproliferation, international safeguarding, and nuclear forensic purposes. The IPF target holder and U-capsule were designed using Solidworks 3-D software. The compilation and analysis of nuclear reaction cross sections from previous experiments involving proton-induced fission of 232Th will be used to evaluate experimental results from cross section measurements conducted at the IPF and the Weapons Neutron Research Facility (WRN) by the Inorganic, Isotope, and Actinide Chemistry group (C-IIAC). The production of alpha-emitting 225Ac via proton irradiation of 232Th is currently of intense interest to the national isotope program [3]. Other radionuclides are unavoidably co-produced along with 225Ac in this process and might be put to beneficial use. Nuclear data collected and analyzed in this work will assist in the dissemination of LANL results to the wider physics community and in managing the complex logistics of radiation safety, radioactive material transport, radiochemical processing, and application of accelerator-produced 225Ac.

**Name:** Albert Liu

**Program:** UGS/Postbacc

**School:** University of Michigan, Ann Arbor

**Group:** MPA-CINT

**Mentor:** Sandberg, Richard L

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25681

# Ptychographic Imaging On A High Harmonic Generation X-Ray Source

Coherent diffraction imaging (CDI), or so-called lens-less imaging, is a novel technique in which the diffraction pattern(s) from a sample is used to reconstruct a high resolution image via iterative phase retrieval techniques. Specific types of CDI have been developed such as ptychography, in which multiple diffraction patterns of the same sample are recorded from overlapping locations on the sample. The overlap of these diffraction patterns makes than phase retrieval more robust than is possible with single diffraction pattern reconstructions. The work detailed in this presentation is focused on the implementation of an automated ptychographic imaging system on a tabletop HeNe laser system that will later be integrated into a high harmonic generation soft x-ray source. Reconstructions were then performed using scripts written in Matlab. Applications of this work are numerous, encompassing the imaging of any objects of interest at nanometer resolution.

**Name:** Brandon Medina

**Program:** UGS/Postbacc

**School:** New Mexico Institute of Mining and Technology

**Group:** P-23

**Mentor:** Younk, Patrick

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25608

# Laser Doppler Velocimetry

Laser Doppler velocimetry, also known as photonic Doppler velocimetry (PDV), is a diagnostic commonly used in shock compression experiments. PDV uses Fourier Transforms to analyze signals from heterodyned laser interferomety to measure velocities in dynamic experiments. The uncertainty in the velocimetry measurements must be well characterized to quantitatively compare experimental results to computational results. That is, we must know which features in the experimental data are statistically significant and which are not. In this presentation, I will discuss the theory and process behind PDV as well as recent work done on understanding the precision, accuracy, and resolution of PDV measurements.

**Name:** Jonathan Morrell

**Program:** UGS/Postbacc

**School:** Massachusetts Institute of Technology

**Group:** ISR-1

**Mentor:** Stonehill, Laura Catherine

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25095

# Radiation Detection in Space Environments with Silicon Photomultipliers

The Cs2LiYCl6:Ce3+ (CLYC) scintillator is sensitive to both neutrons and gamma-rays, and using pulse-shape discrimination (PSD) one can differentiate slower neutron signals from faster gamma-ray signals. This ability to detect neutrons and gamma rays with a single material has wide applications where reduction in the size and weight of a system is of importance, including hand-held instruments and space sciences. Traditionally, PSD is done using high-voltage photomultiplier tubes (PMTs), however recent advances in silicon photomultiplier technology (SiPMs) have made SiPMs a strong candidate for applications requiring PSD. SiPMs are advantageous for space applications because they are small, low-weight and operate at a lower voltage/power than PMTs. The goal of this project was to assess three different SiPMs and select the most suitable for use with the CLYC scintillator on the upcoming SENSER experiment. Important parameters include the PSD characteristics, the energy linearity and the temperature dependence of the SiPMs. Three systems were used to read out information from the SiPMs. A multichannel analyzer (MCA) was used to test the energy linearity because of its excellent resolution. A waveform digitizer was used to verify the results of the MCA and to gain information about the shape of the waves coming from the SiPMs. This would help optimize the PSD parameters to be used with the charge-integrating PSD system, which has a large data acquisition capability to ensure good counting statistics. Analysis tools were written in Python that separated gamma events from neutron events, generated averaged waveforms to gain intuition of the shape of each pulse, and found optimized PSD windows. These tools were first tested with PMT data to ensure their accuracy. All three SiPMs were found to have excellent linearity, and PSD was found to be possible. However, PSD was found to be better with a traditional PMT, as expected.

**Name:** Jayke Nguyen

**Program:** UGS/Postbacc

**School:** University of California at Davis

**Group:** ISR-1

**Mentor:** Hoover, Andrew Scott

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** 15-25858

# GEANT4 Simulation of a Gamma-Ray Detector and its Environment

In a laboratory setting gamma ray detector performance is subject to contamination from scattering off of various laboratory components. Scattering has the greatest influence at keV to MeV level energies, and can significantly increase total detection rate. By running computer simulations using the GEANT4 software (a Monte Carlo code for radiation transport simulation), data was generated for comparison to actual detector readings to account for the scattering of gamma rays. To validate the model, data was collected from cesium-137 with a lanthanum bromide (LaBr3) detector. In the simulation the sources were positioned at a variety of distances, using a variety of energies, to evaluate the fraction of total events from scattering of laboratory equipment. Simulations modeled the environment and detector in detail. For the radioactive source, a simulated gamma ray point source was generated to stand in for the radioactive material. Through the comparison of the simulations and actual data, the amount of scattering off of various lab components was quantified. Additionally, a study was done to determine the influence of adding collimators to the source to understand their effects on reducing scattering.

**Name:** Kimberly Nguyen

**Program:** UGS/Postbacc

**School:** University of New Mexico

**Group:** MPA-CINT

**Mentor:** Sandberg, Richard L

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** 15-25610

# Imaging Polyethylene with Fresnel-Regime CDI Using a Tabletop He-Ne Laser

Coherent diffractive imaging (CDI) is a technique which aims to alleviate issues associated with lens-based X-ray microscopy, such as inefficient light transmission, limited resolution, and lenses that are difficult to produce. CDI can be used in conjunction with an ultrafast pulsed X-ray source in order to achieve nanometer scale spatial and femtosecond scale temporal resolution. In order to resolve such fine details, CDI relies on oversampled diffraction patterns, which are then manipulated via a procedure known as iterative phase retrieval to reconstruct an image of the original sample. This technique typically requires the detector to be placed in the far-field regime in order to obtain a Fraunhofer diffraction pattern, where the wavefront can be assumed to be a plane wave. In near-field Fresnel diffraction, the wavefront on the detector has considerable phase-distortion, significantly complicating the reconstruction algorithm. The farther into the Fresnel regime the detector is placed, the more substantial the phase-distortion. Here, we demonstrated Fresnel-regime CDI using a tabletop HeNe laser, analogous to a coherent X-ray source, and the effects of reconstructing a sample in the Fresnel regime were examined. This tabletop He-Ne CDI setup was further applied to imaging polyethylene samples. Polyethylene is a prominent plastic polymer utilized for a variety of engineering applications from creating packaging materials to joint replacements. Further study is required to understand polyethylene's response to mechanical strain, pressure, tensile strain, and radiation. Studying structural responses under dynamic conditions allows for the refinement of current computational models for predicting polyethylene performance in extreme conditions. CDI offers a possible cost-effective and efficient approach for analyzing polyethylene performance as an engineering material.

**Name:** Raquel Pacheco

**Program:** UGS/Postbacc

**School:** New Mexico Institute of Mining and Technology

**Group:** XTD-PRI

**Mentor:** Sherrill, Leslie Welser

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** 15-25311

# BHR3 Mix Model Sensitivity and Verification

BHR ( Besnard-Harlow-Rauenzahn) is a model designed to calculate the evolution of a mix layer. BHR accounts, in an average sense, for turbulent Rayleigh-Taylor mixing, Richtmyer-Meshkov shock-driven mixing, and Kelvin-Helmholtz shear-driven mixing. Implemented and run in the FLAG radiation hydrodynamics code, BHR3 was tested in simple shock tube geometries which were simulated as an attempt to verify the third generation of the BHR model. 1-D calculations were performed in FLAG using both BHR2 and BHR3 models; the differences of these simulations will be compared in this poster along with simulations testing the sensitivity of initial conditions in both models.

**Name:** Emily Pittman

**Program:** GRA

**School:** University of New Mexico

**Group:** XTD-NTA

**Mentor:** Hagelberg, Carl Richard

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** 15-25536

# Simulating Material Behaviors in Gas Gun Experiments

Gas gun experiments have the potential to investigate material properties in various shock strength conditions, making them a valuable research tool for the development of equations of state and material response under shock loading. Results from these experiments are applicable to many fields. We have used gas gun experiments to assess the capabilities of the Flag hydrocode and equations of state. Our first test gauges Flag's ability to simulate the behavior of Argon gas under varying shock conditions. Much of Argon shock data comes from low-pressure shock tube experiments and from plate impacts on the liquefied, cryogenic gases. Data is insufficient for gas-phase, initial density regimes in the range of 200-500 psi. The Shock and Detonation Physics group performed the experiments and the XTD Safety and Security Group developed Pagosa numerical hydrocode simulations of gas gun experiments with the SESAME equation of state (EOS) to develop a physical understanding of shocked Argon gas. Pagosa is a Los Alamos National Laboratory 2-D and 3-D Eulerian hydrocode capable of modeling high velocity compressible flow with multiple materials. We replicated these simulations in Flag, a Langrangian muliphysics code, using the same materials and parameters included in the Pagosa simulations. The objective of this research was to compare results from the Flag simulations to results from the Pagosa simulations and to experimental data. The results obtained from Flag simulations were consistent with both Pagosa and the experimental data. Our other set of gas gun simulations test Flag's replication of high explosive (HE) experiments with PBX 9501. One simulation was created to model an experiment that measured a Hugoniot point on the overdriven products for PBX 9501 to extend data from which current EOS models draw. We used this calibrated model to design a double-shock experiment involving two sections of HE separated by Tantalum.

**Name:** Katherine Schneider

**Program:** UGS/Postbacc

**School:** Colorado School of Mines

**Group:** AOT-AE

**Mentor:** Bishofberger, Kip A

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25760

# Analysis of Field Uniformity inside Large Transverse Electromagnetic (TEM) Cells

This study simulates electromagnetic propagation in an existing large-scale Transverse Electromagnetic (TEM) cell using CST Microwave Studio to validate current results of RF testing. Driven by a range of frequencies between 10 kHz and 250 MHz, a symmetric TEM cell should generate uniform electromagnetic plane waves to an object under test. Adding asymmetries to the chamber can cause field nonuniformity due to multimoding. This project quantifies several possible field variations. This analysis lends insight to potential limitations of the TEM cell, with opportunities to improve the chamber's utility.

**Name:** Daniel Shields

**Program:** GRA

**School:** Colorado School of Mines

**Group:** P-27

**Mentor:** Tovesson, Fredrik

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** 15-20130

# High-Resolution Correlated Fission Product Studies With SPIDER at LANSCE

The SPIDER detector (SPectrometer for Ion DEtermination in fission Research) has obtained high-resolution, moderate-efficiency, correlated fission product data needed for many applications including the modeling of next generation nuclear reactors, stockpile stewardship, and the fundamental understanding of the fission process. SPIDER simultaneously measures velocity and energy of both fission products to calculate fission product yields (FPYs), neutron multiplicity (nu), and total kinetic energy (TKE). These data will be some of the first of their kind available to nuclear data evaluations. An overview of the SPIDER detector, analytical method, and preliminary results for thermal 235U(n,f) will be presented.

**Name:** Hayley Suitts

**Program:** UGS/Postbacc

**School:** Northeastern Illinois University

**Group:** ISR-1

**Mentor:** Tornga, Shawn Robert

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** 15-25418

# Effect of Atmospheric Dynamics on Photon Propagation

Simulating global performance of hard-radiation detectors for nuclear test-ban treaty monitoring relies on an accurate model of photon transportation. The intensity of a photon signal attenuates as it interacts with elements in the atmosphere. The successful detection of a signal therefore depends on whether or not it traveled all the way to the detector before completely attenuating. Our current simulation tool, DIORAMA (Distributed Infrastructure Offering Real-time Access to Modeling and Analysis), calculates total photon attenuation for nitrogen and oxygen, with the assumption that the atmosphere is static over time with an altitude-dependent density. Current synthesized attenuation data tables omit uncertainties and therefore provide no way to propagate errors in attenuation. DIORAMA incorporates only nitrogen and oxygen in total attenuation and omits all other constituents. Additional variations in density due to diurnal, seasonal, and solar cycle fluctuations are also disregarded. The refinement of our photon transportation model involves including uncertainties for attenuation values, which will provide us with an estimated degree of certainty in the values affected by attenuation. Furthermore, incorporating argon into total attenuation as well as using a dynamic atmosphere that reflects the time-variation of density will yield greater accuracy. The uncertainty values, available in publications of the individual attenuation data tables, were found to have a decreasing exponential dependency on energy. This function provides us with an error in attenuation at any energy. The total atmospheric attenuation that includes nitrogen, oxygen, and argon was calculated as a weighted sum of the constituent atomic attenuations. Space weather data indicates that the densities of these constituents fluctuate enough over time to have a further effect on attenuation uncertainty. We will show, by integrating these effects into DIORAMA code, that the expected signal flux propagated through the atmosphere can vary substantially and has the potential to affect the likelihood of detection.

**Name:** Robert VanDervort

**Program:** GRA

**School:** University of Michigan

**Group:** XTD-IDA

**Mentor:** Mussack Tamashiro, Katie

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** LA-UR-15-25495

# A Diffusive Code, xRage, is Compared to Experimental Data from Omega

A sound speed discrepancy between solar models and data collected using helioseismology exists. The sound speed discrepancy is the most pronounced at the base of the convective zone (CZ) for otherwise consistent solar models. One potential solution is that the opacity models for important elements such as carbon, nitrogen and oxygen are incomplete. At these high energy-density conditions few relevant opacity measurements exist to compare to the models. Only relatively recently have user facilities been able to reach the temperatures and densities that resemble the convective zone base. It is our long term goal to determine the opacities of carbon, nitrogen and oxygen at the relevant conditions. Preliminary testing has occurred at the Omega Laser Facility in Rochester, New York. Presented are the results of the shots taken on April 22, 2015. A half hohlraum was used to drive a supersonic radiation front through a dominantly carbon, CRF, foam. These results are compared to diffusive xRage simulations.

**Name:** Chloe Whittington

**Program:** UGS/Postbacc

**School:** Tuskegee University

**Group:** XCP-5

**Mentor:** Honnell, Kevin Guy

**Category:** Physics

**Type:** Individual Poster

**LA-UR:** 15-25425

# Using a Tabular Equation of State for the Spherical Noh Problem

Verification problems test a computer code's ability to numerically solve a problem with a known exact solution. This is useful because by correctly solving a problem with a known solution, it increases our confidence that it can solve more complex problems for which the solutions are unknown. Here we examine the ability of the xRAGE hydrocode to yield correct results for the spherical Noh problem when using a tabular equation of state (EOS). The one-dimensional spherical Noh verification problem is comprised of a compressible, ideal gas of negligible viscosity that is initialized with a uniform, spherically radially inward velocity. This flow pattern creates an outgoing shock wave at the origin, and is commonly used to assess a code's ability to convert kinetic energy into internal energy at the point of convergence or overcome the "wall-heating effect". The unphysical wall-heating effect results in an underestimate of density and an overestimate of specific internal energy in the calculated answer. Traditionally, the Noh problem is run using an ideal gas EOS; however, in real applications the codes typically use much more complex EOSs represented by tables. Our goal was to implement a tabular analog of the ideal-gas EOS in the Noh problem and evaluate whether or not additional errors arise from interpolating from a table rather than using the analytical formula. Using GRIZZLY, a computer program designed to create EOS tables, we made our own tabular EOS. xRAGE input decks and run scripts for the Noh problem were then edited so it would use the tabular EOS rather than the analytic one. For each version of the Noh problem, the results were compared to the exact solutions and a convergence test was done. The analytic EOS converged 69.9% while the tabular EOS converged 83.9%.