



# Los Alamos National Laboratory

“Championing Scientific Careers”  
Highlighting Student Research

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Student

Symposium

**July 26<sup>th</sup> – 27<sup>th</sup>, 2013**

# 2013 Student Symposium Abstracts

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**Name:** Ayesha Arefin  
**Program:** GRA  
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**Group:** B-10  
**Mentor:** Rashi Iyer  
**Category:** Biosciences  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25782

## **Construction of Biomimic Membrane for Artificial Alveoli**

Chronic Obstructive Pulmonary Disease (COPD) is the third leading cause of death in the United States, claiming more than 124,000 lives in 2007 alone. The current challenge to study this chronic disease requires a reliable in vitro lung disease model. The in vitro lung model should provide effective levels of oxygen and carbon dioxide exchange, alveolar type 1 and 2 cell adhesion, extracellular matrix production, and mechanical properties thus creating an environment for the cells conducive to regular metabolic activity and cellular responses recapitulating the human lung. Recently, microfluidic technology comprising of stacked micro channel networks has been explored to fabricate artificial lungs. However, use of silicon-based membrane and PDMS (Polydimethylsiloxane) membrane does not suitably mimic the functionality of the lung alveoli. Synthetic biodegradable polymer PLLA (poly-L-lactic acid) membrane is widely used to build three-dimensional scaffolds for generation of tissue-engineered organs due to their biodegradability, mechanical properties, and degradation properties. However, the hydrophobic nature of these membranes does not promote cell adhesion. Here, we report the fabrication and verification of ultrathin nanomembranes that aim to maximize gas transfer and cell adhesion efficiency while minimizing membrane-blood contact area. By optimizing the PLLA concentration, spin coating method, and surface chemistry we were able to show that the modified membrane has maximum cell adhesion, proliferation, differentiation, nutrient transfer, and gas exchange capabilities. Our results suggest a potential use of this bio-membrane as a candidate scaffold in the development of an artificial human lung facilitating the understanding of COPD and other lung related diseases.

**Name:** Sarah Barr  
**Program:** UGS  
**School:** University of Portland  
**Group:** B-11  
**Mentor:** David Fox  
**Category:** Biosciences  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-24897

## **Metabolic Engineering in *Synechococcus Elongatus* sp.PCC7002 for Biofuel Production**

Fossil fuels are the primary natural source for the industrial production of most commodity chemicals and fuels. Bioengineering of photosynthetic microalgae towards the production of these compounds is particularly appealing since the process does not compete with arable land nor does it add to the harmful effects of subterranean drilling. Therefore, growth and harvest of fuels from microalgae allow for a large relief from dependence on fossil fuels. We tested the ability to metabolically engineer biofuel production into the cyanobacterium, *Synechococcus elongatus* sp. PCC7002, which is a phototrophic microbe that is readily amenable to genetic manipulation and fast growth thus making it a suitable candidate for production of biofuels. PCC7002 utilizes the methylerythritol phosphate (MEP) pathway to synthesize isoprenoids, which are branched, unsaturated hydrocarbons with combustion properties similar to gasoline and jet-fuel. We hypothesize that increasing carbon flux through the beginning of this pathway will subsequently increase the final isoprenoid yield to sustainable and efficient levels for biofuel applications. Specifically, this study examined the rate limiting conversion of the metabolically abundant substrates, pyruvate and D-glyceraldehyde 3-phosphate (GAP), via 1-deoxy-D-xylulose 5-phosphate synthase (DXS) into 1-deoxy-D-xylulose 5-phosphate (DXP). This represents the first step in the MEP pathway that may generate a number of different isoprenoids, depending on the organism. The *dxs* genes chosen for this study originated from the colonial microgreen alga, *Botryococcus braunii* Race B, which is a prolific producer of isoprenoids but grows too slowly to act as a competitive biofuel source. Our goal was to overexpress the *B. braunii* *dxs* genes in PCC7002 through genetic manipulation in order to increase isoprenoid production while also maintaining fast growth rates. Efforts towards this include DNA vector design, PCC7002 culturing and maintenance, and genetic manipulation. Isoprenoid production in both the wild type and transformed strain were examined using gas chromatography (GC).

**Name:** MariJo DeAguero  
**Program:** UGS  
**School:** Northern New Mexico College  
**Group:** B-10  
**Mentor:** Elizabeth Hog-Geller  
**Category:** Biosciences  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25432

## **Reinforcement of the Sentinels of Innate Immune Defense to Contain Infection**

In an attempt to find strategies for public health protection, different approaches are used to provide a solution for prevention of infectious diseases. All currently available antibiotics target essential bacterial processes and thus contribute to the evolution of drug resistant microbes. Development of antimicrobials that inhibit host processes essential for microbial virulence is a novel approach that avoids selective pressure driving drug resistance.

Phagocytosis is a process in which cells engulf a foreign organism, such as bacteria, and digests it to protect the body from the spread of infection.

This defense mechanism is not always successful. Some pathogens find a way to manipulate phagocytic cells and use them as a transport system to spread infection throughout the body. Here we present a study on the role of two host factors, the protein kinase PKC $\eta$  and its substrate MARCKS (myristoylated alanine-rich protein kinase C substrate), in phagocytosis and pathogen survival. We have chosen virulent *Burkholderia thailandensis* as a model organism for this study due to its highly antibacterial-resistance and ability to survive within professional phagocytic cells, such as macrophages. We have validated the key role of PKC $\eta$ -MARCKS interaction in *Burkholderia* phagocytosis using various techniques such as gene function knockdown via RNA interference, cell imaging analysis, Western blot and Enzyme Linked Immunosorbent Assay (ELISA). The results from this study will advance our understanding in essential host-pathogen interactions that can be applied for development of novel antimicrobials.

**Name:** Michelle Earley  
**Program:** GRA  
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**Group:** T-6  
**Mentor:** Bette Korber  
**Category:** Biosciences  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25576

## **A Look at Adenovirus as a Vector for an Effective HIV Vaccine**

The human immunodeficiency virus (HIV) epidemic has become a major global public health issue affecting millions worldwide. The key to overcoming HIV is to develop an effective vaccine, which has proven to be a great challenge. Because adenovirus serotype type 5 (Ad5) vectors have been known to induce strong HIV-specific T cell immune responses, they were recently used in two phase IIB vaccination clinical trials (STEP and HVTN 505), focusing on the efficacy of the vaccines in high-risk individuals. The STEP study was designed as a double-blind, multi-center, randomized, placebo-controlled trial in North America where the participants were stratified based on their Ad5 neutralizing antibody levels, higher levels indicating pre-existing immunity to the virus. Unfortunately, the trials were stopped early as they showed a larger number of HIV infections within the vaccinated group, specifically Ad5 seropositive individuals, than the placebo group. Because of these negative results, it may be beneficial to examine other types of Adenoviruses. There are seven types of human adenoviruses, HAdv-A through D, and since adenovirus neutralizing antibodies are specific to each type, it is important to examine and understand the different types. A few important characteristics to study are cross-reactivity (the reaction between an antigen and an antibody that was generated against a different antigen), phylogeny (evolution and diversity), and epitope coverage. Using tools developed by Bette Korber and her team at LANL these characteristics are being examined for 32 different proteins found in five different adenoviruses (human adenoviruses 5, 35, 26, 4 and chimpanzee adenovirus).

**Name:** Eric Generous  
**Program:** GRA  
**School:** John Hopkins University  
**Group:** D-3  
**Mentor:** Alina Deshpande  
**Category:** Biosciences  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25277

## **Monitoring of Dengue Fever Using Wikipedia**

The early detection of outbreaks is vital for protecting against and mitigating the impact of infectious diseases. Traditional surveillance systems typically rely on clinical data that can take up to weeks to report, often much too late to be of use for early detection. This problem is exacerbated in developing nations, which often lack the medical infrastructure to properly track disease incidence. Internet based data sources, most notably the use of internet search queries and Twitter, have been shown to be useful for monitoring diseases in near real time. This project expands upon this work by demonstrating the use of data from Wikipedia a data source not previously utilized to track Dengue in Thailand and India. By examining the number of hits on certain pages on the Thai and Hindi Wikipedia websites, it was possible to monitor the incidence of Dengue in near real time. The time series generated from the Wikipedia data was validated and shown to be accurate (correlation greater than 0.8) in comparison to both Ministry of Health reported clinical cases and Google Dengue Trends, an internet search query surveillance system. This study has demonstrated that Wikipedia data can be used to monitor the incidence of dengue and could prove useful for tracking diseases in areas or countries with limited surveillance resources.

**Name:** Martin Loncaric  
**Program:** UGS  
**School:** Harvey Mudd College  
**Group:** T-6  
**Mentor:** Sandrasegaram Gnanakaran  
**Category:** Biosciences  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25575

## **Modeling the Enzymatic Degradation of Cellulose**

Biofuels are an important field of research today because of their potential impact on energy and national security. Corn is currently the most widely used crop to produce ethanol because of its high sugar content. However, this approach is disadvantageous because it competes for food and leaves the bulk of the crop to waste. It would be much more practical to turn cellulose into biofuels, since it accounts for approximately 50% of plant matter by mass. Several organisms, such as termites and fungi, break down cellulose into glucose using enzymes, although this could take weeks to years. Industrial attempts to produce biofuels with such enzymes require hours to days, with the added financial cost of the enzymes. This research focuses on making the industrial process more economically viable. Prior studies have made advances in this field, especially with regard to the synergistic combination of endo- and exocellulases – two types of enzymes which break down cellulose faster when working together. My research involved improving a stochastic model [1] and creating a system of differential equations for understanding the mechanistic aspects of the degradation of cellulose. I will then compare the results of the two models to each other and experiments in order to determine when to use the less computation-intensive differential equation model. Finally, I will use both models to determine whether time-dependent addition of enzymes could accelerate the degradation process.

[1] Asztalos, Andrea; Redondo, Antonio; Gnanakaran, Sandrasegaram

**Name:** Aaron Roybal  
**Program:** UGS  
**School:** University of New Mexico  
**Group:** ENV-ES  
**Mentor:** Philip Fresquez  
**Category:** Biosciences  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25676

## **The Extent of Tritium Levels and Migration From Area G**

Area G is the Laboratory's primary low-level radioactive waste site since 1957. Wastes are buried in pits, trenches, or shafts and then covered with fill material. Tritium ( $^3\text{H}$ ), an isotope of hydrogen that follows the water cycle, is one of the main contaminants in waste materials at Area G and has been consistently detected in annual environmental monitoring studies of soils and plants. The purpose of this study was to determine the extent of  $^3\text{H}$  at subsurface depths using overstory vegetation from (1) set points around the perimeter of Area G, (2) the maximum source over time (1996 through 2013), and (3) the highest sources as a function of distance from the perimeter fence line. Juniper trees are excellent indicators of subterranean  $^3\text{H}$  migration. As such, approximately three pounds of tree branch tips were collected from 13 trees at various set points around the perimeter of Area G at chest height. Also, tree samples (three each) along two transects radiating outward from the south side of Area G were collected. All samples were analyzed for  $^3\text{H}$ . Results show that all  $^3\text{H}$  concentrations in trees around the perimeter of Area G were detectable (where the result is higher than the total propagated uncertainty at three sigma; the 99% confidence level) and higher than the regional statistical reference level (RSRL) ( $>0.74$  pCi/mL). The highest  $^3\text{H}$  concentration ( $2.6\text{E}05$  pCi/mL) was detected from a sample that was collected on the south side of Area G nearest the tritium shafts; although, it was the highest recorded level over the period of record, the levels were still below the screening level for radionuclide dose to plants. Finally, based on the two transect studies, the levels of  $^3\text{H}$  decreased with distance.

**Name:** Kirstie Swingle  
**Program:** UGS  
**School:** University of New Mexico  
**Group:** MPA-CINT  
**Mentor:** Gabriel Montano  
**Category:** Biosciences  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25784

## **Lipopolysaccharide-Membrane Interactions Explored Using Lipid Bilayer Assemblies**

Lipopolysaccharides (LPS) are found in the outer membrane of gram-negative bacteria and provide stability for the bacteria. LPS is also known to be an endotoxin that can penetrate human cells and induce responses such as toxic shock that can result in death. Understanding the mechanism of LPS interaction with membranes is crucial in making advances in understanding such pathogenic effects and developing therapeutics. Lipid Bilayer Assemblies (LBA) can be used as model systems for investigating membrane interactions and responses. In this study, lipid bilayer assemblies were formed using lipids of varying properties and LPS from different species were introduced. Different ion concentrations (i.e.  $\text{Ca}^{2+}$  and  $\text{Na}^{+}$ ) in the presence of LPS were also screened to evaluate LPS-membrane interaction as a result of electrostatic conditions. Depending upon LPS, lipid and environment, a variety of membrane responses were observed such as lipid tubule formation, holes in the lipid bilayer assembly or formation of lamellar sheets that appeared to be mobile. These results indicate that a number and combination of conditions can impact the mechanism of LPS-membrane interaction and are under continued exploration. A detailed understanding of such interactions will allow for refined mechanisms of LPS interaction for the biomedical community and aid in design of therapeutics and biosensor design. The results also indicate promise in using LPS in soft-lithography approaches for biomaterials design and are also being explored as such.

**Name:** Robin Yoshida  
**Program:** UGS  
**School:** Saint Anselm College  
**Group:** B-10  
**Mentor:** Taraka Dale  
**Category:** Biosciences  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25611

## **Testing a Pipeline for Improved Outdoor Performance of Algae**

Algal biofuel has become a popular area of interest as the need for a cleaner, greener, and more sustainable fuel source becomes more apparent. Growing algae for biofuel has shown to be a promising path to significantly reducing the use of fossil fuels. Harvesting algae for fuel presents many benefits, including minimal land usage to grow, high yield, and algae's unique ability to grow in a variety of conditions like salt water or desert land. Ongoing research is being carried out to make this new source of energy a viable option. One challenge is that algae populations have shown some inconsistencies when taken out of a controlled lab setting and introduced to outdoor environments to grow. In order to better understand this problem and conserve resources, we aim to develop a pipeline for characterizing a given strain, predicting its outdoor performance, and validating that performance using climate-simulated growth conditions. To this end, our collaborators predicted the most ideal geographical locations and months to grow our example strain of algae, *Picochlorum*, sp. Then, using a script with light and temperature data from the predictions, we mimicked the environment in Phenometric environmental photobioreactors (ePBRs). We grew the algae under these conditions, and the results will be presented here. We will be able to apply these methods to different strains of algae, to give more accurate and consistent predictions about the overall lipid and biomass production potential they have. This will help ensure that future money spent on outdoor ponds will achieve maximum efficiency.

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## **Stabilizing Lipid Bilayers through Photopolymerization**

Lipid bilayers have long been prepared and studied as models of cell membranes. Uses for these bilayers include, but are not limited to, surface functionalization for bioassays and biodetection. However, the weak intermolecular forces between the individual monomeric lipids in the bilayer have proven to be a limitation due to structural instability when subjected to conditions such as extended storage, removal from water, or exposure to surfactants. By photopolymerizing the bilayer through exposure to UV light, our hope is to strengthen bonds through cross-linking. Once successfully polymerized, the bilayer, composed of bis-SorbPC, should be inherently more stable and available for short term storage or labeled for use in biodetection assays. Advantages of photopolymerization include the bilayer's retention of fluidity, while increasing long term stability. Use of these stabilized bilayers for detection on the waveguide sensor will be beneficial as it will not only decrease the time needed for detection of a marker, but increase the sensitivity, stability, and accuracy when compared to other surface coating techniques.

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## **Re-Establishment of Analytical Chemistry Techniques to Support Am-241 Production**

Historically, Americium-241 ( $^{241}\text{Am}$ ) has been produced and analyzed by a variety of sites across the Department of Energy (DOE) Complex. Currently, there are no DOE sites that produce  $^{241}\text{Am}$  for use in well-logging neutron sources ( $\text{AmBe}$ ), as ionization sources in smoke detectors, and low-energy (59.5 keV) gamma-ray sources for material/coating measurements.

In previous production efforts, few standards for isotopic and chemical purity were reported as being available. Hence, a focus of this project will be to develop or re-establish techniques to ensure >99%  $^{241}\text{Am}$  isotopic purity and >95%  $\text{AmO}_2$  chemical purity as well as plutonium (Pu) content, Pu isotopics, trace element,  $^{237}\text{Np}$  (neptunium) and U (uranium) content measurements. This project will support bulk production of  $^{241}\text{Am}$  and will support the development of certified reference materials as a collaborative project with the National Institute of Standards and Technology (NIST) and the DOE New Brunswick Laboratory (NBL).

To accomplish these goals, this project will address the re-establishment of thermal ionization mass spectrometric (TIMS) methods for isotopic and chemical purity of Am content in addition to existing methods for Pu. The TIMS measurement will be corroborated with other methods, such as non-destructive analysis (NDA) by gamma-ray spectrometry. The trace element,  $^{237}\text{Np}$ , and U analyses will be performed using inductively coupled plasma – atomic emission spectroscopy (ICP-AES) and ICP-MS techniques. By re-establishing and developing techniques for chemical and isotopic purity, there are also applications toward future efforts relating to “forensic” determinations and tighter material specification standards. The results from TIMS and gamma-ray spectrometry measurements will be presented.

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## **Improved Sample Utilization in TIMS Isotopic Ratio Measurements**

Thermal Ionization Mass Spectrometry (TIMS) has served as the “workhorse” in the isotopic ratio determination of nuclear materials for decades and is widely regarded as the benchmark for such analyses; however, TIMS methods for the assay of actinide systems are hindered by poor ionization efficiencies/sample utilization. Enhanced performance is achievable by refining the development and application of existing porous ion emitter (PIE) technologies as TIMS ionization sources. PIEs have exhibited improved sample utilization, permitting the use of lower sample quantities during isotope ratio measurements. Existing literature serves as a solid foundation for work to exploit the enhanced efficiency associated with PIEs to develop a novel set of chronometric approaches to investigate young materials with exceptionally low  $^{230}\text{Th}/^{234}\text{U}$  ratios and to establish relatively non-exploited chronometers, such as the  $^{228}\text{Th}/^{232}\text{Th}$  ratio of interest in sub-40 year old samples. I will also work to extend existing capabilities to measure the  $^{235}\text{U}/^{231}\text{Pa}$  chronometer of value in the analysis of enriched materials. Opportunities will be evaluated that further advance PIE construction to produce ion sources better able to ionize actinides of interest.

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## **Quinoxolinon Salen Ligands for Spectrophotometric Molecular Recognition**

A resurgence of interest in actinide science and actinide chemistry has been inspired by a need to address the potential for environment contaminations through a nuclear waste spill in the environment. There are many techniques to detect actinides from environmental samples such as inductively coupled plasma, potentiometry, x-ray fluorescence, kinetic phosphorimetry, and colorimetry. While these techniques can be very sensitive they are often not portable or inexpensive, delaying the need for on-site real-time data. Spectrophotometry is a promising area as an Ultraviolet-Visible (UV-Vis) spectrometer can be small, low-cost, and portable. At present, there are ligands that will bind to uranyl and give a unique signal, however, competing metals such as copper can interfere with that signal.

Our group has previously developed a Quinoxolinol salen ligand. This ligand was used to determine selectivity of uranyl over other metal ions. Computational chemistry is becoming an invaluable tool in the understanding of reaction intermediates and pathways, as well as excitations and vibrations caused by atoms interacting. Computations using ground state and excited state time-dependent density functional theory (TDDFT) indicated ligand-metal charger transfer bands as the cause in the shift in the absorbance from the ligand in the UV-Vis. The ligand was modified by changing the substituents on the phenyl ring that included electron donating and electron withdrawing groups, as well as changing the binding site from a 2N 2O to a 4N, 5N, and 5N 1O site, to tailor the excitations to increase the selectivity in the UV-Vis without overlapping the absorbance bands of the ligand, copper complex, and uranyl complex.

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## **Probing the CN Bridge of the Actinide Cyanometallates**

The alkali and alkaline earth metal tetracyanoplatinates were reported two centuries ago, yet, few compounds have been reported in the actinide square planar cyanometallate class of compounds,  $An_x[M(CN)_4]_y$ .<sup>1</sup> The  $D_{4h}$  idealized symmetry of the square planar tetracyanoplatinate anion allows for platinumophilic interactions that manifest as columnar structural features in the solid state.<sup>2</sup> Utilizing this structural feature provides a new means for probing the chemistry of the 5f elements. Described here is the synthesis, emission, Raman spectroscopy, small molecule XRD structural characterization, and DFT calculations of the recently reported actinide cyanometallates, general formula  $An_x[M(CN)_4]_y$ .

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## **Extraction Chromatography Resin for Rapid Separations in Post Detonation Scenarios**

In a post detonation scenario, it is essential to acquire the most information about the device and transgressors as soon as possible. One way to achieve this information, is to separate out some key fission products for nuclear forensic analysis. Since extraction chromatography allows rapid, reliable, and selective separations it makes this technique a prime candidate for nuclear forensic analysis. For this reason extraction chromatography resins DGA and UTEVA, which are commercially available through Eichrom Industries, were characterized for the purpose of rapid separations. These resins show promising separation factors based off previously reported results. The elements which have not been previously well characterized were analyzed by performing batch contact studies and the  $k'$  values for varying acid matrixes and concentrations were determined. An ideal separation flowsheet was developed for the separation of a dissolved hybrid glass/cement bead and was fashioned after previously published data and assumptions based on trends which will be discussed. Depending on detection compatibility, all eluents were analyzed by either a NaI well detector or the inductively coupled plasma – atomic emission spectroscopy.

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## **Thermal Stability of Ammonium Nitrate/Aluminum Mixtures**

Ammonium nitrate (AN) /aluminum (Al) mixtures have become prevalent in homemade explosives around the world. Ammonium nitrate, a white crystalline solid at room temperature, is a common fertilizer, but is also a good oxidizing agent used in explosives. Both AN and Al are easily accessible ingredients, making this mixture a fairly easy one to create. Aluminum, an electropositive metal that is highly reactive in powdered form, is a common fuel ingredient in energetic materials that provides enhanced energy release over organic fuels. Aluminum powder is stable at lower temperatures due to a strong, uniform oxide coating that inhibits further oxidation of the core aluminum. Recently, there have been many questions raised as to whether or not these ammonium nitrate /aluminum mixtures have problems remaining stable in humid environments. The purpose of this project is to test the thermal stability of different mixtures of ammonium nitrate and aluminum and evaluate the effect of different impurities within the mixture. Controlled impurities include water (pH of 7-8), silicone oil, nitric acid (pH 2), and sodium hydroxide (pH 13) which will each be combined with a mixture of ground ammonium nitrate and aluminum powder. The effects of these impurities will be evaluated with various thermal analysis techniques including differential scanning calorimetry (DSC), vacuum-thermal stability (VTS), and automatic pressure tracking adiabatic calorimeter (APTAC).

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## **Maintaining Optical Properties of Ultra-Short Single Walled Carbon Nanotubes**

Single walled carbon nanotubes (SWCNTs) are a commodity with many potential applications; ranging from composites to electronic transistors to biological sensors due to their remarkable physical, electrical, and optical properties. One of the difficulties of incorporating SWCNTs into many systems is their polydispersity in length and electronic properties. In this study, we attempt to control length effects by cutting SWCNTs with various techniques. Difficulties arise if the cutting technique is too aggressive, creating over-functionalization, which quenches optical properties. The overall goal is to maintain individual SWCNT properties in a tube on the order of 20-100 nm. To characterize our results, we employ photoluminescence emission spectroscopy (PLE), absorption spectroscopy (UV-VIS), and atomic force microscopy (AFM).

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## **Chemical Forensic Science**

The entire nuclear fuel cycle is a chemistry-intensive process, from accessing the raw materials from ore, to enriching and forming the fuels, to the eventual long-term disposition or reprocessing of the spent fuel. This chemistry is vital to forensics, as the chemical history of a sample imbues it with unique signatures that should provide insight beyond the scope of information that standard methods such as morphology and isotopics provide. Uranium oxides can be easily oxidized and tend to react with their surroundings over time, which necessitates the assessment of what new chemical signatures are introduced by the aging of a sample. To accomplish this, the analysis of a series of both high-purity standards and commercially prepared samples aged under conditions controlled for temperature and humidity has been undertaken. We have used complementary chemical (XANES, XRD, etc.) and morphological (SEM) characterization techniques to help provide a more robust catalogue of the signatures contained within the aged oxide samples. Results to date show an increased oxidation rate in higher humidity and higher temperature samples, with the oxidation products being  $\text{UO}_3$  hydrates. Furthermore, it appears that the commercially prepared samples oxidize faster than the higher-purity standards.

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## **Sanitary Effluent Reclamation Facility Waste Product as a Concrete Amendment**

Various projections for the volume of waste generated during operations of LANL's Sanitary Effluent Reclamation Facility (SERF) and the costs associated with the waste disposition have indicated a need for exploration of alternative disposition pathways. The intent of this project is to use this LANL waste product—a sludge cake principally comprised of magnesium and iron silicates with minor amounts of calcium carbonates and aluminum oxides—as a replacement for fly ash in cement and concrete formulations. Processing steps to transform SERF sludge into an acceptable cement amendment include: washing, milling, reacting sludge with supercritical CO<sub>2</sub> and subsequent calcining. Analyses have been conducted to determine residual chloride in sludge waste, and particle size following milling; elemental analysis to assist in cement mix design; Powder X-ray Diffraction has been used to study mineralogy; and compression testing of cast concrete samples has determined concrete performance. Processed SERF sludge appears to provide a concrete amendment suitable for the replacement of fly ash.

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## **Probabilistic Computing for Graphics Processing Units (GPUs)**

Probabilistic computing provides alternatives to traditional deterministic approaches. Probabilistic computing probabilistically calculates or probabilistically guesses and then calculates data leading to a close-to-correct answer. The goal of this research is to develop flexible and efficient probabilistic algorithms that support analysis of large-scale data on the new exascale architecture. Developing these algorithms so they are usable and generic will enable others to use the algorithms in other contexts. This project involves extension and modification of probabilistic computer algorithms designed to run on GPUs for fast processing of large data sets. The original project at LANL, Top K, found the top K elements in a list by taking a sample of values and iteratively splitting the data into bins using a guess and check procedure to determine whether the Kth element is in the middle bin. The second program, K-D tree, uses the prior Top K work to perform a multidimensional space partitioning. This is also easy to check for correctness and is useful for finding certain qualities like nearest neighbor. In top K and K-D tree programs we use probabilistic computing because it makes the program faster. Implementation of these programs has required development of C++, Linux, CUDA, and Thrust programming skills. Thrust is the library that communicates with the GPU, and it provides a higher-level interface to the GPU that makes programming easier. Results include implementation of a probabilistic KD-tree algorithm on a GPU and improvement of the K-D tree program by finding bugs and writing code to make the program more efficient. The K-D tree program has been expanded to four dimensions. Future research will explore different ways to partition the arrays and make the program more efficient. This work is part of collaboration between HPC and CCS.

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## **SEFI- A Soft Error Fault Injection Framework**

As the high performance computing (HPC) community continues to push for ever larger machines, reliability continues to be a serious obstacle. Further, as feature size and voltages decrease, the rate of transient soft errors is on the rise. HPC programmers of today have to deal with these faults to a small degree and it is expected this will only be a larger problem as systems continue to scale. Therefore we present SEFI, the Soft Error Fault Injection framework, a tool for profiling software for its susceptibility to soft errors. In particular, we focus in this paper on logic soft error injection. Using the open source virtual machine (QEMU), we demonstrate modifying emulated machine instructions to introduce soft errors. We conduct experiments by modifying the virtual machine itself in a way that does not require intimate knowledge of the tested application. With this technique, we show that we are able to inject simulated soft errors in the logic operations of a target application without affecting other applications or the operating system sharing the VM.

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## **Simplification of Optimization: A GUI Approach to MADS**

Model-based decision making related to environmental management problems is a very challenging problem. There have been substantial theoretical research and practical applications related to this problem. However, there are very few cases in which the actual decision analyses have been tested in the field to evaluate their adequacy. Over the last several years, we have performed a series of decision analyses to support optimization of a monitoring network at Los Alamos National Laboratory (LANL). The problem dealt with actual contaminant transport in the regional aquifer beneath LANL. At three separate stages, the existing monitoring network was augmented based on analyses of the existing uncertainties; in total, five new monitoring wells were proposed. At each stage, the data collected at the new monitoring wells demonstrated the adequacy of the uncertainty quantifications and the decision analyses.

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## **Control Systems Security**

A Control System is a device that gathers data and uses it to monitor and control a process. Since many Control Systems in use today were developed long before networks, they were designed for functionality, reliability, safety and physical security – not cyber security. Since Control Systems require security to ensure that these devices within them are maintaining functionality and are completing their actions properly a field called Control Systems Security is necessary. Control Systems Security is used in a wide range of applications to protect Control Systems from vulnerabilities and the Control System from being compromised. Control Systems Security can be implemented in multiple ways depending on how the Control System is set up. Control Systems Security can be used to manage complex computer systems or to handle management of waste water systems. A Control Systems Technology Lab was created as an Institutional resource to check compatibility, maintainability, and security of a Control System by using the tools within the Control Systems Technology Lab in combination with equipment brought by the Control System Customer. It will also be used for training, vendor interactions and a common place for the LANL Control System community to interact.

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## **PyDac: A Resilient Run-Time Framework for Divide-and-Conquer Applications**

Heterogeneous many-core architectures that consist of big cores and small cores promise a good balance between single-thread performance and multi-thread throughput. Such systems impose challenges on the runtime system design. One such challenge is the reliability of the hardware and it is likely that the runtime system will need to contain faults and reduce the chance of a fault from propagating.

We propose a Python-based run-time framework called PyDac. PyDac supports a two-level programming model based on the divide-and-conquer strategy. This framework isolates all of the data that a small core is working on. Therefore, a faulty small core can be reset independently and the task restarted. To test this run-time, an unconventional heterogeneous architecture consisting of PowerPC and ARM cores was emulated on an FPGA. We demonstrate feasibility of this runtime design with Strassen's algorithm.

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## **Visualizing CO<sub>2</sub> Sequestration Plumes and Leakage Regions**

Geologic CO<sub>2</sub> sequestration involves pumping CO<sub>2</sub> into underground reservoirs to reduce its prevalence in the atmosphere. CO<sub>2</sub>-PENS is a model built using the GoldSim framework that is used to run various CO<sub>2</sub> injection cases. It is especially useful because of how fast it is able to run a large number of injection scenarios. The CO<sub>2</sub>-PENS results viewer is a Java GUI (Graphical User Interface) that allows the CO<sub>2</sub> leakage outputs of CO<sub>2</sub>-PENS to be visualized with relative ease. This work describes modifications and improvements made to the results viewer. Several key problems with the existing viewer were identified and fixed, along with numerous other small bug fixes. Additionally, a multitude of other features were added for increased capability and to make the GUI more user-friendly and accessible.

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## **Efficient Program for Plotting Particle Size Distribution**

Plutonium-238 heat sources have provided electrical power to numerous United States space programs. The fuel's chemical and physical stability as an oxide ( $^{238}\text{PuO}_2$ ) coupled with its relatively short half-life of about 88 years makes it a primary candidate for the radioisotope thermoelectric generators (RTGs) installed on long-term space missions. Because it is an actinide, however, this efficient fuel also poses multiple health and safety risks to the environment and human populations; the most common and dangerous concern is the inhalation of small particles of  $^{238}\text{PuO}_2$ . These particles range down to fractions of microns in diameter, so it is imperative that particle size distributions of fuel samples be measured. In this process, images are taken of a sample of particles and subjected to computer analysis to measure the areas of individual particles, and to calculate and plot the cumulative volume and differential histograms. The current programs used at LANL can take up to 30 minutes to process the information of large batches of information; therefore, this project requires a simple, efficient program to process and graph the desired information in a quick and reliable manner. The ParticleData program allows the user to select the input file, as well as the bin diameter increment size and scale for plotting (linear or logarithmic). It then produces a graph including the cumulative and differential plots of the relative volumes of the particles in the sample. This graph can then be used to evaluate the distribution of particles in the fuel sample for health and safety hazards, and production control.

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## **Automation of the CDC Hardening Process**

During my summer with DCS-3 and the CDC (Central Distribution Center), I have experienced the amount of effort that is put into hardening (new) incoming computer prior to deployment in accordance with the Los Alamos National Laboratory's requirements. Over the course of the summer, I have noticed much of the work done by this team is manual and can be done in a more efficient fashion. Efforts are being made to automate many of the processes, omitting much of the manual and repetitive (labor-intensive) procedures. Instead of manually recording customer, order and other information for every machine that is received by the CDC, we are developing code and processes which will utilize a machine's Package Tracking Number to find other information about the machine/order that is needed to continue the hardening process. To achieve this, we have obtained information from two data feeds. Both of the data feeds we have chosen each have information specifically needed by the CDC to allow the machine to be processed. The old manual process is expected to be shortened with the emergence of this new automated procedure.

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## **Control of an External Microcontroller Using the Android Operating System**

There is a critical need for rugged and portable control systems for field-deployable sensors. Since the Android is an open-source operating system, a smartphone can potentially be modified to serve as a communications device to interface with a controller and many types of experiments/sensors in the field. The communications can be wireless or via USB cables. Through this project, we have demonstrated two-way communication and control of an external Arduino microcontroller, as well as real time data acquisition, through an easy to operate GUI on an Android OS phone operating through Bluetooth wireless communication.

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## **To Hash Meshes in Small Places**

We examine the potential of using hash-based algorithms to improve spatial operations required for unstructured meshes on Graphics Processing Unit (GPU) architectures. We investigate the performance of hash-based methods on Central Processing Units (CPU's) relative to a typical binary tree method and compare the speed of hashing on the GPU to the CPU. We implement memory optimizations which exploit the nature of the mesh allowing for compression of the data structure. The hashing method is then extended from a perfect hash to a compact hash using open-addressing. These implementations are tested across a variety of GPU architectures on both a randomly generated sample mesh and on an existing cell-based Adaptive Mesh Refinement (AMR) shallow-water hydrodynamics scheme.

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## **History of Supercomputing at Los Alamos**

Our goals have been to compile a history of supercomputing at Los Alamos National Laboratory, to exhibit that history in a comprehensible way, and most importantly to provide a centralized framework for ongoing documentation. The project included recording conversations with retirees and employees who have had long careers in supercomputing at the lab, thereby establishing the beginnings of an oral history archive. We gathered as much raw data as could be obtained on the specifications and performance of every supercomputer at Los Alamos since the laboratory's founding. We created an index that lists and tags all of the primary documents we acquired for the project, to which new entries can be added indefinitely as the project continues into the future.

Finally, we built the prototype of an exhibit with the goal of making that history accessible to the casually interested, and to provide an interface through which others can contribute their knowledge to the project. The exhibit prototype was designed using Ruby on Rails to create an interactive website as the front end to a SQLite database of supercomputer information.

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## **Co-Design Summer School 2013**

Exascale computing presents an enormous opportunity for solving some of today's most pressing problems, including clean energy production, nuclear reactor lifetime extension, and nuclear stockpile aging.

To solve many of these problems, multiscale strategies that combine molecular dynamics (MD) applications with hydrodynamics solvers at the macroscopic level are employed. We studied and optimized such an application on a heterogeneous research cluster with an eye toward scalability at the exascale level. In order to achieve higher performance, we take advantage of adaptive mesh techniques to dynamically coarsen the tasks and reduce the number of high latency MD simulations. We further decrease execution time by exploiting multiple runtime systems and programming models to maximize throughput and increase the utilization of the cluster. Finally, we explored various tools and techniques to increase resiliency and usability.

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**LA-UR:** 13-25204

## **Open Source Virtual Environment System**

Open Source Virtual Environment System: CAVELib is a software application programmer interface (API) used for LANL to support the Virtual Reality (VR) environment implemented in the CAVE and RAVE. CAVELib is used to create interactive three-dimensional environments; it handles the details of the CAVE's software including operating system, display system and virtual interaction. However, CAVELib's features are limited to its own libraries and don't provide many options for extending to new interface devices. The purpose of this research is to find an open-source virtual environment system that supports not only the same capabilities as CAVELib but provides expanded features with the ability to implement different user owned libraries. Virtual Reality User Interface (VRUI) is an open-source toolkit developed by Oliver Kreylos, a computer science professor at the University of California Davis. VRUI provides a Virtual Reality Toolkit to develop immersive 3D intuitive applications from the particular configuration of VR environment; applications can be developed quickly and in a portable and scalable fashion, meaning that they are written without a particular input environment in mind and can run on laptops with a touch pad, over desktop environments with special input devices and over VR environments with single-screen and multi-screen tiled display walls or CAVEs. As a low-level toolkit, CAVELib doesn't provide source-code which would allow for writing an application once, and running it in VR environments with widely differing input environments without purchasing additional licenses. On the other hand, VRUI as a high-level semantic interface, supports an easy to program menu system, it treats every environment, even desktops, as immersive environments; while CAVELib would need an instance of the software on every machine running it. The development of this project will allow us not only to create a more robust software with more capabilities for the programs running in the CAVE and RAVE but it will also lead to new discoveries in the use of new technology and the integration of these features to the virtual reality environments.

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**LA-UR:** 13-25614

## **Image Analysis at Scale**

We have implemented a Hadoop based distributed platform for large scale image analysis. Our platform represents segmented images as graphs in a graph database and uses machine learning techniques to identify user specified objects in an image. The software stack consists of the Think Aurelius Titan graph database with Apache HBase as its storage backend. This software has been installed on the Data Intensive Super Computer (DISC) and tested to determine whether our approach will scale well. Testing is performed on every component of the software stack to determine the basic performance characteristics of DISC and the overhead associated with various tasks.

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**Type:** Group Poster Presentation  
**LA-UR:** 13-25555

## **Verification Problems for xRAGE Radiative Hydrodynamics Code**

New solutions were derived for the radiative hydrodynamics equations of a gamma law ideal gas given in Coggeshall [1991]. These solutions were derived by assuming a velocity distribution of the form  $u(r, t) = a*r/t$ , where  $a$  is a constant. The radiation flux was assumed to be non-divergent.

The analytic solutions were then implemented as test cases in the xRAGE radiative hydrodynamics code developed at Los Alamos National Laboratory. By comparing the results of the xRAGE numerical solver with the discretized versions of the analytical solutions, we were able to verify the accuracy of specific xRAGE modules.

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## **Effects of Drought and Heat on Tree Growth and Phenology**

Increased drought and climate warming are a concern for the health of terrestrial vegetation throughout the world. It is widely known that drought leads to the death of vegetation. Trees and forests remove, or sequester, an important part of the human-caused CO<sub>2</sub> emissions from the atmosphere that contribute to climate change through their growth. Climate change, especially heat and drought, could stress trees, reducing their growth and ability to sequester CO<sub>2</sub> from atmosphere. Understanding how plants respond to climate stress will help us quantify potential effects of climate change on forest carbon sequestration. The SURvival and MORTality (SUMO) experiment at Los Alamos National Lab is designed to expose trees to drought and heat stress, eventually leading to death, using rain-out structures to catch water and large chambers to heat the trees. Phenology is study of the timing of certain behavior or growth response in biological organisms. At the SUMO experiment, we measured the growth and phenology of two tree species: Juniper (*Juniperus monosperma*) and pinyon pine (*Pinus edulus*) to study the effect of climate stress on trees. Growth of pinyon pine was much more affected by the drought and heat treatments than the junipers during the duration of the study, which have shown little growth this year. Drought stressed junipers produced more male pollen cones than junipers which received normal precipitation, yet heating minimized this effect. Pinyon pine trees showed very little sign of reproductive growth during the study period. Overall we found that growth of pinyon pine is highly sensitive to the heat and drought stress. Our results demonstrate that drought and heat have the potential to reduce the ability of trees and forests to remove atmospheric CO<sub>2</sub>, potentially diminishing their climate regulation service to humanity.

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## **Solid and Dissolved Phase Aluminum in Storm Water Runoff on the Pajarito Plateau**

Aluminum is the most abundant metal and the third most abundant element found in the earth's crust after oxygen and silicon. It is never found free in nature and is found in most rocks, particularly igneous rocks. It is primarily found in stable silicate mineral phases such as feldspars and phyllosilicates. Aluminum enters environmental media naturally through the weathering of rocks and minerals. In these forms aluminum is bound strongly and is not toxic to aquatic organisms. However, aluminum hydroxide ( $\text{Al}(\text{OH})_3$ ) is somewhat toxic to aquatic organisms. This form of aluminum is common when acid mine drainage is treated and neutralized but is rarely present in a typical environment. Storm water samples collected on the Pajarito Plateau contain measurable aluminum concentrations. The updates by the New Mexico Environment Department (NMED) to New Mexico aquatic life water quality criteria for aluminum are now based on total recoverable aluminum in a sample that has been filtered to minimize the non-toxic mineral phases. This pre-filtration step was suggested by the NMED because total recoverable procedures using unfiltered samples will likely measure significant concentrations of larger particulate mineral phase forms of aluminum that are not toxic, yet the typical "dissolved" metal fraction might exclude some amorphous or colloidal aluminum fractions that can be toxic. This study is designed to aid in the determination of appropriate filter pore size needed to partition the non-toxic mineral phases of aluminum from the potentially toxic forms of aluminum. This partitioning will be evaluated by comparing the results using varying filter pore sizes.

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## **Automated Facility Layout Generation for Nuclear Power Plants**

My proposal is to test whether or not automated layout planning software, originally developed for the microelectronics industry (B\*-Tree Floorplanner), pronounced “b-star-tree”, (Chen and Chang, 2006), can be re-purposed to aid in the layout of industrial facilities. The purpose of creating multiple automated layouts is for the creation of synthetic imagery. The Benchmark Imagery project seeks to create a suite of real and synthetic imagery of overhead images of industrial facilities to test geospatial algorithms. The goal is to create synthetic images, which will appear realistic to both algorithm and human. The methodology included two tasks. The first task was to perform background research into nuclear power plant layouts. The next task was to obtain three-dimensional (3D) models of nuclear power plants. Then we created an input file for B\*-Tree Floorplanner. The input file contained information about the 3D models and their adjacency/connectivity to the other models. B\*-Tree Floorplanner produced ten different layouts. The layouts generally exhibit an east-west or a north-south orientation. All ten iterations can be utilized for facility layout. Deciding which layout to use is based upon two criteria. The first is whether the layout is conducive to producing electricity. The second is the environment where the nuclear power plant is built. We have demonstrated that B\*tree can be used as a way to automate facility layouts. The multiple layouts from B\*tree will be used to create synthetic images which was our over-arching goal.

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## **Assessing the Validity of Magnetic Field Model TS05 with Geomagnetic Storm Data**

Earth's magnetic field, generated by molten metallic currents in its core, has been measured continuously since the 1960s. Satellites are placed at geosynchronous orbit (6.6R<sub>E</sub>), in the region where the magnetic field shifts from being produced internally to externally, making them sensitive probes of the global current structure and dynamics. Empirical field models are developed from these data and other input parameters. However, since extreme conditions are infrequent, the soundness of models during storm events has not been thoroughly tested. The purpose of this study is to evaluate the strengths and limitations of TS05, the most successful magnetic field model compared to GOES data. The inferred magnetic field directions from the TS05 model are first compared to storm events measured by GOES-8 through -12, replicating the results of Huang (2008), and then validated by repeating the analysis on an independent dataset.

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## **X-Ray Reflectivity and Diffraction of ALD Calcite Thin Films in Air and in Water**

Carbonates are one of the most abundant groups of minerals in earth systems and are important in many geological settings and industrial processes. Calcite ( $\text{CaCO}_3$ ) thin film produced by atomic layer deposition (ALD) offer a new method to evaluate the surficial properties of carbonates as well as interactions at the carbonate-fluid interface. Using synchrotron X-ray reflectivity and X-ray diffraction, these films are observed to be porous, polycrystalline, and have crystallites oriented with the major (104) calcite cleavage plane parallel to the surface of the z-cut single crystal quartz substrate. An  $\text{Al}_2\text{O}_3$  buffer layer, present between quartz and the calcite film, does not affect the as-deposited film, but does influence how the films reorganize in contact with fluid. Without a buffer layer, calcite reorients its crystallites to have populations (006) and (030) parallel to the substrate, while those with  $\text{Al}_2\text{O}_3$  become more amorphous. Due to a higher percentage of pore spaces available for fluid infiltration, films deposits at higher temperatures make the calcite thin films more susceptible to amorphization. These films are chemically similar, but structurally dissimilar, to bulk natural calcite. Nevertheless, they can be a complementary tool to traditional single crystal reflectivity studies on carbonates, particularly for important but less common minerals, to evaluate mineral-fluid interfacial interactions.

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## **Investigation of Total Electron Content Variation over Thunderstorms**

Solar and geomagnetic activity are considered to be the main drivers of ionospheric variation, but recent findings have suggested that tropospheric weather could also have a significant effect in terms of tides, generation of atmospheric gravity waves, and seeding of spread-F. A recent study has shown anomalous fluctuations nearby large mesoscale thunderstorms in the U.S. Great Plains [Lay et al., GRL 2013]. In this study, we examine GPS TEC data from a ground-based GPS receiver located at Los Alamos National Laboratory during the summer of 2012 and further analyze Great Plains data to clarify the connection between nearby thunderstorms and anomalous TEC variations. The LANL GPS TEC receiver uses a Kalman filter based program developed by Carrano et.al (2009) to determine the TEC by measuring the phase shift between the L1 and L2 GPS frequencies. We use the World Wide Lightning Location Network and the Los Alamos Sferic Array as an indicator of nearby thunderstorm activities.

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## **A Mega-Fire's Hydrologic Impacts on Nutrients Concentrations in Stormwater & Soils**

A Mega-Fire's Hydrologic Impacts of Burn Severity on Nutrient Concentrations in Surface Water Runoff and Soils  
Las Conchas Fire, Jemez Mountains, New Mexico

Climate change is currently exhibiting intensified wildfire behavior and severity conditions in the Southwest. Following large fires, or mega-fires, surface water runoff and soils contribute high concentrations of nutrients to water bodies and has the potential to impair surface water quality in urban and rural environments. Although there is a considerable amount of research on the effects of nutrients in surface water runoff and soils following a fire, the need to investigate mega-fire conditions on nutrient levels transported from various fire severity classes is required. The purpose of this study is to investigate the contributions of nitrite-nitrogen (NO<sub>2</sub>-), nitrate-nitrogen (NO<sub>3</sub>-) and orthophosphate (OP) levels in surface water runoff originating from various wildfire severity classes from the Las Conchas fire in the Jemez Mountains, New Mexico. To complete this task, NO<sub>2</sub>-, NO<sub>3</sub>-, and OP concentrations will be determined from surface water runoff and soils originating from qualified high, moderate, low, mixed, and control (unburned site) fire severity types. Fire severity site qualification was determined using geospatial applications and a simple linear regression model in a previous study. We hypothesize that our results from the high severity burn area will have the least contribution of NO<sub>2</sub>-, NO<sub>3</sub>-, and OP and control will have the highest.

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**LA-UR:** 13-25232

## **Climate Change Increases Physiological Stress of Two Southwest Tree Species**

Climate change is expected to cause widespread forest mortality due to the strain of heat and drought affecting tree physiology. The Los Alamos Survival Mortality Experiment (SUMO) implements treatments simulating powerful effects that may occur over the next century with climate change; including a 50% precipitation removal and +4°C temperature increase. Due to atmospheric demand for water, trees exchange water for carbon dioxide to perform photosynthesis. Stomatal conductance is the measurement of water loss from tree foliage and is highly sensitive to changes in atmospheric demand and tree water availability associated with decreased rainfall and increased temperature. Trees in this semi-arid climate, including the piñon pine (*Pinus edulis*) and the one-seed juniper (*Juniperus monosperma*) we studied, use various strategies to hold on to as much water as possible. A LI-1600 Steady State Porometer was used to measure stomatal conductance along with photosynthetically active radiation (PAR) and leaf temperature. Five treatments are present for both tree species at the SUMO site: ambient, ambient control, drought, heat, and drought+heated. The data reveals that stomatal conductance decreases as time of day progresses, as leaf temperature increases, and as PAR increases; and increases as average water potential increases. The preliminary results indicate an overall decrease in stomatal conductance with a greater effect on piñon pine than one-seed juniper due to stresses of drought and heat during the month of June, the driest and warmest month at SUMO.

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## **Urban Storm Water Runoff on the Pajarito Plateau**

Under the national pollutant discharge elimination system (NPDES) Individual Permit, Los Alamos National Laboratories monitors storm water discharge from solid waste management units (SWMUs). Storm water is monitored below SWMU's for pollutants associated with legacy discharges and to measure performance of sediment mitigation structures established to control runoff. In many cases, storm water emanating from upstream landscapes flows onto SWMUs transporting sediments and pollutants not associated with the SWMU and contributes to the runoff loading. Target action limits (TALs) are defined for the 450 SWMUs within the 250 site monitoring areas (SMAs). Previous studies have shown that concentrations of copper, zinc, aluminum, gross alpha particles, and polychlorinated biphenyls (PCB's) in storm water runoff on the Pajarito Plateau have, in many cases, exceeded those TALs. Often, these constituents are not associated with SWMUs and instead are associated with more naturally occurring materials and urban runoff.

The purpose of this study is to determine the contribution of pollutants in storm water running-on to SMAs adjacent to urban and industrial environments. Global Water automated sampler's were deployed and are currently maintained on a regular basis throughout the monitoring season and storm water samples are collected, analyzed, and assessed for potential contaminants. This will help determine whether SWMUs were contributing pollutants to canyon bottoms or if other sources were contributing to the chemical character of the SMAs storm water runoff.

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**LA-UR:** 13-25626

## **Computational Study of Variable Stars and the Kepler Satellite**

The Kepler satellite was launched on March 6, 2009 with the primary mission to detect Earth size planets orbiting stars through transits. The Kepler satellite is also perfect for the detection of variable stars. Since stars are laboratories for plasma physics, the study of variable stars allows us to study stellar structure and evolution. The Kepler satellite collects the light curves of stars in 3 months long quarters. Currently, the light curves of 1849 stars from 14 quarters of Guest Observer data are being analyzed for variability. Data reduction programs to reduce noise levels and Fourier Transforms are used on these star's light curves. The transform is the integral limit of fitting a light curve with many sine waves of arbitrary frequencies, amplitudes, and phases. The component frequencies resolved by the Fourier Transforms help classify stars. Based on the pulsation periods and the amplitude of the pulsations, the stars are classified as being non-variable or pulsators such as  $\gamma$  Doradus,  $\delta$  Scuti, hybrids showing characteristics of both  $\gamma$  Doradus and  $\delta$  Scuti stars, or other types of variable stars including binary star systems and star spots on rotating stars.

Hybrid  $\gamma$  Doradus and  $\delta$  Scuti stars are of interest for asteroseismology because the dual modes of pulsation probe the entire star. Because hybrid pulsations are driven by two exclusive mechanisms, they are expected to occupy a small region of temperature and luminosity in the Hertzsprung-Russell diagram. Kepler shows a large number of hybrid pulsators. Our work to categorize these stars is the first step to learn what is different between stellar models and real stars.

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## **Determination of Hydraulic and Mechanical Properties of Fractured Rock**

Investigating CO<sub>2</sub> reactive transport processes is crucial for understanding mechanisms of carbon sequestration and shale gas extraction during hydraulic fracturing. In addition, geomechanical studies analyzing the integrity of caprock material is important to determine sealing capacity in sequestration and fracture propagation in shale gas development. To date, many studies have been conducted to measure the properties of core samples from storage or shale sites. However, very few experimental data are available for fractured rock permeability and the dynamic behavior of fluid flow during mechanical failure. This study aims to collect experimental data on mechanical and hydraulic properties of anhydrite and Utica shale gas samples. A tomographic triaxial coreflood system (TCS) is used to measure the Young's modulus, Poisson ratio, permeability and strength for each core sample prior to fracturing. After mechanical failure, we investigate the flow of CO<sub>2</sub> and CO<sub>2</sub> rich-brine through the fractured rock sample at T=50 °C and P=2,000 psi. We examine the dissolution and mineralization processes induced by CO<sub>2</sub> and the brine solution, and characterize mineral surfaces following the experiment. We will use tomography to characterize fracture patterns and apertures of damaged anhydrite and shale. Some experiments will be conducted using in situ x-ray tomography that will allow determination of fluid (CO<sub>2</sub> and H<sub>2</sub>O) distribution within fractures.

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## **Temperature Dependence of Lithium Cation-Exchange in a Geothermal Reaction System**

Geothermal energy is a widespread natural and renewable resource and is especially common in the western United States. Geothermal reservoirs that have enough natural permeability to be economically viable are limited, so in the early 1970s a team of scientists at Los Alamos National Laboratory pioneered the use of hydraulic fracturing to create such reservoirs for the generation of thermal energy. To evaluate the commercial potential of an EGS reservoir, it is useful to estimate the amount of surface area available for heat transfer created by stimulation. A robust method of determining the surface area in EGS reservoirs has not been developed to date. An ongoing study at LANL is evaluating the use of the lithium (Li) ion to estimate surface area in these systems based on the concept that the amount of cation exchange of Li should be proportional to surface area. Presently, Li tracer is being used at an EGS demonstration site at Newberry Crater, OR. To interpret field tracer tests, the proportionality between surface area and cation exchange must be understood. Laboratory cation exchange capacity and batch sorption parameters were determined for Li using water and minerals similar to those found at Newberry Crater. Dynamic flow-through column experiments under reservoir conditions (125°C- 225°C) were also performed to compare with the batch results. The column experiments at temperatures ranging from 125°C to 275°C indicated a strong temperature dependence of Li cation exchange, with the exchange parameters obtained from the room temperature batch experiments significantly underestimating Li retardation in the columns. We also performed a room temperature lithium flow-through experiment, and Li retardation in this experiment was consistent with the cation exchange observed in the batch experiments. These results show the importance of performing laboratory tests at the temperatures expected in the field to accurately predict field tracer behavior.

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## **Developing a Robust Trace Element Analysis Method for Geological & Nuclear Materials**

A trace element is a chemical element that makes up less than 0.1% of a geological or nuclear material. Trace element abundances are useful signatures for understanding the source and history of a material. Complex sample matrices (e.g., Si-rich or U-rich) make collection of quality trace element data a challenge. We have developed two sample preparation methods: 1) HF-HNO<sub>3</sub> digestion and 2) Na-peroxide sintering and a six point external calibration with internal standardization inductively coupled plasma mass spectrometry (ICP-MS) method for determination of trace elements in geological samples. For trace element measurements, we utilize a Thermo Element XR double focusing magnetic sector ICP-MS equipped with a cross-calibrated discrete dynode secondary electron multiplier and Faraday detector, which in combination make it possible to measure analyte isotopes in low ( $m/dM = 300$ ), medium ( $m/dM = 4,000$ ), or high mass resolution ( $m/dM = 10,000$ ) modes across twelve orders of magnitude of linear dynamic range (i.e., ppq to low weight%).

New trace element data will be used to better understand the geological origin of Rare Earth Element (REE) bearing eipsyenites in the Caballo and Burro Mountains of New Mexico. REE have a wide range of applications including automotive pollution catalysts, energy storage, medical isotopes and national defense. The geological origin of eipsyenites is enigmatic- they may have been emplaced as magmatic dikes, or formed by the interaction of potassium-rich fluids with granitic basement rocks. The results of this work will help clarify the general REE resource potential of eipsyenites, will improve our understanding of eipsyenite formation/emplacement and their REE enrichment, and will provide useful insight for future exploration of similar domestic REE deposits. Preliminary results thus far suggest that eipsyenites are formed by potassium-metasomatism. New trace element data collected in this study will provide insights into the origin(s) of the metasomatizing fluids.

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## **Monitoring Sensitive Bat Species at Los Alamos** **National Laboratory**

Bats play a critical role in the ecosystem and are vulnerable to disturbance and disruption by human activities. In recent decades, bat species in the U.S. and elsewhere have decreased tremendously. There are 47 different species of bat in the U.S. and 27 of these occur in New Mexico with 15 different species documented at Los Alamos National Laboratory (LANL) and surrounding areas. In 1995, a four year study was initiated at LANL to assess the current status of bat species of concern, elucidate distribution and relative abundance, and obtain information on roosting sites. There have been no definitive studies since then. Biologists in the Environmental Protection Division at LANL initiated a multi-year monitoring program for bats in May 2013 to implement the Biological Resources Management Plan and to comply with Federal laws and regulations related to sensitive species. The objective of this on-going study is to monitor bat species abundance and richness over time at LANL. The spotted bat (*Euderma maculatum*) is listed as “Threatened” by the State of New Mexico and is known to occur at LANL. Four other species of bat are listed as “Sensitive” and also occur here. Bat species abundance and richness was measured using an acoustic bat detector, the Pettersson D500X. This ultrasound recording unit is intended for long-term, unattended recording of bat and other high frequency animal calls. The detector was deployed at two locations at LANL to determine the presence/absence of bat species. Study sites were selected based on proximity to water where bats may be foraging. Bat calls were analyzed using Sonobat, software that can help determine specific species of bat through their calls. A list of bat species at these sites was developed and compared to lists from 1995-1998. Future studies will be implemented based on these findings.

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**LA-UR:** 13-25630

## **Predicting Ground Motion from Injection-Induced Seismic Events**

Among the methods proposed for carbon sequestration is subterranean carbon dioxide injection. Suitable locations for this type of sequestration include former hydrocarbon reservoirs, like those underlying the Kimberlina area near Bakersfield, CA. However, injecting fluids like carbon dioxide into the subsurface changes the ambient stress state, which, in turn, can fracture rock or activate a pre-existing fault and induce earthquakes. As such, observation and public perception of these earthquakes have jeopardized fluid injection projects in the past, emphasizing the importance of understanding how a specific location will respond under certain earthquake magnitude and distance conditions. Regression models have been developed that, for a specific location, consider the distance to an earthquake's source, the earthquake's magnitude, and site amplifications to develop equations that may be used to model ground motion. In this project, a program was written that considers the ground motion prediction equations (GMPEs) presented in Douglas (2013), as well as the site amplification equations from Abrahamsen (2008) and Boore (2008). This program has a range of applications, including site-response curve generation for user-specified site conditions, as well as plot generation for suites of magnitude/distance combinations and VS30 ranges. This program will be instrumental in developing further models of a proposed Kimberlina injection site, which will ultimately be used to assess the seismic hazard associated with fluid injection in the greater Bakersfield hydrocarbon play.

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**LA-UR:** 13-25485

## **Motion Planning for Manipulators Under Uncertainty**

Automation of robotic systems is an active area of research. This poster deals specifically with path, or motion, planning of robots. Path planning is the construction of a path that will allow the robot to go from point A to point B (the goal) in a given environment successfully. In this case, successfully means reaching point B without collision. Many different path planners have been developed over years. The most effective path planners assume the system dynamics, environment, and sensors are perfect, but this is generally not the case in real world problems. Adding in uncertainty of any type increases the complexity of the problem. In addition to uncertainty, applying the path planning problem to a high dimensional robot, such as a seven degree of freedom (DOF) manipulator, creates the “curse of dimensionality” and many problems become nearly impossible to solve in real-time. The purpose of the research presented here is to develop a path planner that can be implemented in real time by a high DOF (i.e. 7-10 DOF) manipulator in an uncertain environment. In order to accomplish this goal, we are using a sample-based path planner combined with a probability map of the environment (that characterizes the chance of collision with an obstacle) to find a path that optimizes a cost function. The cost function used here minimizes both the chance of collision and the length of the path the robot will execute to reach the goal.

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**Category:** Engineering  
**Type:** Individual Poster Presentation  
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## **Mass vs. Volumetric Flow Rate. The Discrepancy in the ASME AG-1 HEPA Standard**

The American Society of Mechanical Engineers (ASME) AG-1 code defines HEPA filters as having “a minimum efficiency of 99.97% when tested with an aerosol of essentially mono dispersed 0.3 micrometer diameter test aerosol particles,” but it does not clarify a measurement procedure for the flow rate through the filters. Both actual cubic feet per minute (ACFM), which measures a volumetric flow rate and standard cubic feet per minute (SCFM), which measures a mass flow rate are mentioned in the code, with no distinction made between them. This can be problematic in air flow applications. For example, if a system was maintaining 1000 SCFM through a typical HEPA filter, the flow measured by ACFM would vary by 15% at a temperature change from 40 to 115 degrees Fahrenheit. A cooperative test plan with a DOE audited facility (Air Techniques International Inc., Owings Mill, MD) will determine a set of correction factors for ACFM and SCFM flow measurements. The elevation difference between the two test locations is fundamental for the test. The LANL Aerosol Engineering Facility has had an aerosol wind tunnel since 2006, but some modifications were necessary to accommodate the test procedure. Due to the need of many sampling configurations and locations, the test procedure was semi-automated with three control valves synchronized with an optical particle counter through LabView software. To achieve accurate single point sampling, an in-line mixing unit was developed which is nearing a patent application. Many considerations and modifications were necessary before even beginning HEPA efficiency testing. Our wind tunnel nearing optimization and we are close to generating data.

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## **Electromechanical Actuation System for X-Ray Generator**

The Dual-Axis Radiological Hydrodynamic Test platform (DARHT) creates three-dimensional (3-D) X-Ray images. It accomplishes this by firing electron beams perpendicular to each other, passing each beam through a metal plate, creating orthogonal X-Ray images which can be overlaid to create a 3-D X-Ray. To allow for multiple shots to be completed sequentially with minimal delay, a revolving cylinder is used to rotate each material sample into place. Rotation is accomplished by a linearly actuated arm, which pushes tangentially against ratchet teeth which have been machined into the cylinder's rim. The motor pushing the arm is a direct current (DC) brushless servo motor which communicates through a microcontroller to the operator's computer by way of American Standard Code for Information Interchange (ASCII). An issue arises, however, due to the imprecise motor movements of DC servo motors, which causes the cylinder to rotate unpredictably. Furthermore, the feedback methods employed to deduce exactly when such errors occur are impaired by the cumbersome weight of ASCII interfaces. Thus, an electromechanical redesign for the entire X-Ray actuation system was needed. The updated design consists of increasing torque available from the motor, improving the precision by using a DC stepper-motor, replacing ASCII control architecture with digital input-output architecture, and implementing new and improved feedback controls and switches to assist operators and engineers in the field.

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## **Secure VoIP on Session Border Controller**

Acme Packet enables service providers to deliver trusted, first class interactive Communications-voice, video and multimedia sessions-across IP network borders. Net-Net session border controllers (SBC) satisfy critical security, service assurance and regulatory requirements in wire line, cable and wireless networks. The Deployments support multiple applications-from VoIP trunking to hosted enterprise and residential services; multiple protocols-SIP, H.323, MGCP/NCS and H.248; and multiple border points-interconnect, access network and data center. Net-Net SBCs secure the VoIP in different facet but we will focus on layers security with diverse protocols and the high availability (HA) in case of event failure, the HA design guarantees that no stable calls are dropped . Furthermore, the Net-Net SBC HA design provides for full media and call state to be shared across an HA node. The solution uses a VRRP-like design, where the two systems share a virtual MAC address and virtual IPv4 address for seamless switchovers. The DoS protection for autonomic, SBC self-protection against malicious and non-malicious DoS attacks and overloads at Layers 2 to 4 (TCP, SYN, ICMP, fragments, and so on) and Layers 5 to 7 (SIP signaling floods, malformed messages, and so on). ). AT the layer 3 and 5 the session-aware access control for signaling and media using static and dynamic permit/deny access control lists (ACLs). The complete infrastructure topology hiding at all protocol layers for confidentiality and attack prevention security. Service infrastructure DoS prevent per-device signaling and media overload control, with deep packet inspection and call rate control to prevent DoS attacks from reaching service infrastructure such as SIP servers, softswitches , application servers, media servers or media gateways.

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## **Active Q-Switching in NMR Applications**

Climate change has resulted in unusually high temperatures affecting existing forests by decreasing water absorption. A tree's ability to sequester carbon and produce oxygen depends on the water content of that tree, and by measuring the water content of the trees, we are able to more accurately determine the health of forests and build better climate models. Low-field NMR offers a means of determining the water content in trees in vivo. The system applies an oscillating magnetic pulse, tilting the axis of the proton spins in the subject, and a receiver coil picks up the signal resulting from the proton precession. For the best data, a large signal is needed accompanied by a short ringing time following the pulse. This is because, depending on the quality (Q) factor of the circuit, ringing can be a problem as the signal can only be recorded after the system completes its ring down time. During this ring time, data from the signal is lost, effectively reducing the signal to noise ratio. In order to combat these losses, the signal needs to be maximized while simultaneously reducing ring time. A high Q factor results in a large signal but also significant ring time, and a low Q factor gives a smaller signal but minimal ring time. Combining the needed qualities of these two factors requires the use of Q-switching. Using LTspice, we simulated how the Q-switch would dampen the ringing. Without any damping, the signal produced by our coil rings for five milliseconds. With the Q-switch integrated into the circuit, ring time was significantly reduced, down to one millisecond. When the Q switch is turned off, the precession is detected by the high Q circuit, maximizing the signal to noise ratio.

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## **MiniMAX: Miniature, Mobile, Agile X-Ray System**

We present the design of a unique, lightweight, compact, low-cost, x-ray system: MiniMAX (Miniature, Mobile, Agile X-ray) along with typical radiographic data obtained in our trials. This system exploits the best aspects of Computed Radiography (CR) and Digital Radiography (DR) technology. In contrast to a conventional, flying-spot scanner, MiniMAX records a photostimulated emission-image from a CsBr or BaFBr:Eu storage phosphor using a single flash from a bright, red LED filtered through an extremely efficient ( $OD > 9$ ) dichroic filter. When combined with compact, sealed, radioisotopic x-ray source (eg.  $^{57}\text{Co}$ ,  $^{75}\text{Se}$ ,  $^{99}\text{Ir}$ , or  $^{60}\text{Co}$ ), the complete system weighs less than 6 lbs and is suitable for inspecting sealed containers, facilities, and cargo. Because digital images are made immediately available, these can be readily uploaded and analyzed on a tablet computer.

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## **Natural Gas Network Flow Optimization**

Natural gas is used to heat homes and to power gas-turbines in power plants which produce electricity. Sources of natural gas are often separated by great distances from the loads. As a result, there are major gas pipelines that run across states and across countries. Laws of physics that govern the steady-state flow through these pipelines dictate that the square flow is proportional to the difference in square pressure between the ends of a pipe and inversely to the length of the pipe. We consider networks with tree structures, which closely resemble the structure of major interstate pipelines in the US. Given a fixed input flow, the remaining flows on the tree are uniquely determined based on the loads. Since it is not uncommon for pipeline lengths to exceed 10,000 miles, to prevent pressure from dropping too much it is necessary to install compressor stations along the pipe which locally boost the pressure, making it feasible to transport the gas over such long distances. However, there is an operational cost associated with running the compressors that depends on their compression ratios: the ratio of outlet to inlet pressure at the compressor. Different configurations of compressor ratios might lead to feasible pressures that support the flows, but some are more expensive than others. The goal is to find an optimal configuration that minimizes the total cost of running the compressors while maintaining feasible pressures. We propose two ways to solve this optimization problem efficiently. The first method is based on reformulation of the problem as a geometric program, and the second is based on a well-known dynamic programming approach. We plan to apply both these methods to the Belgium gas network and to the US Transco pipeline, which runs from the Gulf of Mexico up to Pennsylvania, and compare their performance.

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## **Assessing the Durability and Robustness of O-Rings Used in SAVY-4000 Containers**

The SAVY-4000 container system has been developed to replace the Hagan-type containers used to store radioactive material in the vault for extended periods of time. The lifetime limiting factor for these containers is a Viton-based O-ring, and current procedures do not require the replacement of these O-rings. The O-rings will deteriorate when exposed to increased temperatures and when in the presence of radiation, however the damage to the O-ring from repeated openings and closings of the container is unknown. The durability lifetime of this O-ring was explored by systematically opening and closing each of four SAVY one-quart containers 100 times while performing helium leak testing periodically. The leak rates after the 100th open/close cycle were about a factor of 4 higher than the initial leak rates; however the final leak rates were still 3 orders of magnitude below the failure criterion.

This study also explored how the accumulation of dust or hair on the O-ring surface would affect the leak rate of the containers. Results indicated that the presence of a single hair that extends from the exterior of the container to the interior of the container would cause the seal to fail by an order of magnitude. When the O-ring was intentionally coated with either standard Arizona road dust (5 $\mu$ m particulates) or silica gel powder (37-63 $\mu$ m particulates), the O-ring failed the leak testing criterion by 2 orders of magnitude. However, the act of dropping and rolling the O-ring around in an area contaminated with dust and hair did not cause the O-ring to fail, even though dust and hair were present on the O-ring.

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## **A Pneumatic Transfer System for the National Critical Experiments Research Center**

For some time, there has been a programmatic need to perform measurements of short-lived isotopes in irradiated samples. Samples can be irradiated at the National Critical Experiments Research Center (NCERC) at the Device Assembly Facility (DAF) on the Nevada National Security Site (NNSS) using the four critical assembly machines: Planet, Flattop, Comet, and Godiva. Due to their nature, detectors cannot be placed inside the buildings that house the critical assemblies. The time required for ingress and egress to and from the buildings, along with sample movement procedures, do not allow for the measurement of the short-lived isotopes. Therefore, a pneumatic sample transfer system has been proposed to rapidly transfer and position samples to and from the critical assemblies and detectors. The time requirement to transfer the sample from the reactor to the detector is less than one second. In 2013, a memorandum was established to detail the design requirements and facility interface requirements for the rabbit system. Subsequently, designs have been developed for the transfer capsule, in both high-purity polyethylene and reactor grade graphite, and the minimum bend radius was calculated for the tubing. In August 2013, the design team intends to irradiate ethylene propylene and silicone o-rings for their activation potential, impurities, and feasibility for use as seals for the transfer capsules.

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## **Responsive Energetic Sol-Gel-Polymer Nanocomposites for Artificial Photosynthesis**

A variety of photosynthetic organizations can be found in nature. In a majority of such complexes, membrane embedded proteins serve as scaffolds for pigments generating energetically, spatially ordered assemblies resulting in efficient light-harvesting, energy transfer and charge separation. The ability to mimic the efficiency of natural photosynthetic systems has been a goal in biomaterials design for decades. Mesostructured and mesoporous silica made using sol-gel processing are promising host templates for encapsulation of biomolecules and creating bio-inspired assemblies. The sol-gel process involves the transition of a solution system from a liquid "sol" (colloidal) into a solid "gel." Surfactants are commonly used as templates in creating mesostructured or mesoporous silica during the sol-gel process resulting in ordered arrays. In this study, amphiphilic diblock copolymers that form micelles are being investigated as templates for forming mesostructured silica and as composite materials for creating bio-inspired artificial photosynthetic assemblies. We have designed nanocomposites that incorporate porphyrin-based chromophores and carbon-based nanomaterials in varying compositions into responsive block-copolymer micelle assemblies encapsulated in sol-gel in order to generate photo-responsive bio-inspired materials. The designed nanocomposites investigated are an initial attempt to generate responsive, ordered arrays capable of performing artificial photosynthetic processes such as light-harvesting, energy transfer and charge-separation.

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## **Dryseal Special Form Capsules**

A Special Form Capsule (SFC) is a container that is designed for the storage of radioactive sources. There are currently three models being utilized by the Off-Site Recovery Project (OSRP) Group; however, there has recently been a need for longer and larger in diameter SFC models. As a product of these larger models, an increase in mass results in a larger dynamic force during the required drop test per ANSI N43.6. These larger dynamic forces consist of greater loads during drop tests which through impact and vibration make it difficult to seal existing SFC designs. The Dryseal SFC design was proposed as a solution.

These new SFCs utilize NPTF Dryseal Pipe Threads. The NPTF (National Pipe Taper Fuel) thread is designed to provide a leak tight seal without the use of sealing compounds. The roots of both internal and external threads are truncated slightly more than the crests. By torquing the threaded assembly, the sharper crests are crushed into the opposing roots while the thread flanks are drawn together. Thus, there is a complete mating profile making a leak-proof connection without the necessity of a sealing compound. In turn, this "Dryseal" will eliminate the need of the plug currently used in the older SFC models.

This work is to conduct preliminary ANSI N43.6 suitability tests on the proposed Dryseal SFCs. Testing included documenting the torque values necessary to create a leak tight seal, leak testing, drop testing and furnace testing. Upon achieving reliable test results, a final model design satisfying all NRC specifications is proposed.

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## **Improved Geo Registration Using Peak Likelihood Error Minimization**

This project develops a series of algorithms for accurately locating and tracking an object in three-dimensional space (collectively known as geo registration) for implementation on a gimbal-based imaging system. Previous work on geo registration relied on a priori knowledge of the kinematics of the object to be tracked or complex algebraic transformations. The proposed method uses an estimated parameter to eliminate the a priori requirement and attempts to minimize the least-squares error of a Taylor approximation to determine the trajectory and recover the location at any time  $t$ . Using these trajectory approximations, a latency compensation calculation attempts to predict the position of the target and the gimbal body at a future time, recognizing the time delay between the signal origin and action by the gimbal servos measured as the time required to rotate to a new position. Error was incorporated into the latency calculation as an adjustment on the peak likelihood angles at the prediction time. Continuing work will involve developing empirical latency and error functions for the specific gimbal system and processing real signals to confirm simulated results.

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## **Rossi Alpha Integration and Modernization for LANL** **Critical Experiments**

The Rossi Alpha method is used to determine prompt neutron lifetimes in a nuclear fissioning, neutron chain reacting system at or near delayed critical. Knowledge of prompt neutron lifetime is important for a critical assembly as the prompt neutron lifetime is a major contributor to the dynamic system behavior. The Rossi Alpha method analysis uses a mathematical representation of neutron population developed by Richard Feynman in the 1940's. Using the knowledge that neutrons appear in fission chains rather than as single entities, the neutron population in a fissioning system is described by Feynman's equation which discriminates between correlated and accidental pairs of neutrons. Early Rossi Alpha determinations used gating circuits to track the correlated neutrons in a single chain, but modern technology allows for digital time stamping of neutron pulses such as is used in the various LANL custom designed list-mode modules (PATRM systems, etc.). These compact data collection systems remove the need for the bulky complex circuitry used in the 1940's allowing researchers to focus on data analysis.

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## **Lithium Purification Methods for Heat Pipe Applications**

The Department of Energy (DOE) is funding a solar thermal energy program to develop high temperature liquid metal heat pipes for concentrated solar power (CSP) applications. Heat pipes are devices of very high conductance that are suitable for supplying heat to an electrical power plant as well as removing heat from collectors of the CSP system. These high temperature heat pipes must be filled with an alkali metal working fluid in order to reach very high temperatures and last a long time. Lithium, the least reactive element of these metals, exhibits properties that allow it to be used as the high temperature and high performance coolant needed to fill these particular heat pipes. The vacuum distillation and gettering with active metals purification methods are needed to remove the impurities (primarily nitrogen and oxygen) found in lithium to prevent corrosion in the Niobium and Tantalum heat pipes.

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## **Technical Case for Removal of Baseline Pressure Measurements**

The purpose of this work was to develop a technical case to remove initial baseline container inspections required by the DOE-STD-3013-2012 Stabilization, Packaging, and Storage of Plutonium Bearing Materials. Pressure indication of the nested 3013 containers is accomplished by digital radiography and must be completed within 30 days of packaging. The radiographs show the air gap between the nested containers, decreases in this distance indicate container pressurization. Using a photo editing software, the gap for 151 containers was measured. Each container was imaged 12 times taken in 30 degree increments around the container. The average distance between containers was determined. Blind duplicate measurements confirmed the precision of the measurement process.

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## **Compilation of Historical Electrorefining Data at Los Alamos National Laboratory**

Los Alamos National Laboratory's actinide processing support group has begun an effort to retrieve and consolidate historical data pertaining to the plutonium electrorefining process. The electrorefining operation has been run at Los Alamos since the mid sixties, and continues to be run today to produce high purity, alpha-phase plutonium metal for use in defense programs. Data is being retrieved from a variety of locations and consolidated into a single database for use in ongoing studies and process optimizations. Process results and trends can be analyzed with respect to a variety of process parameters (salt system, plutonium electrolyte, back electromotive force, collected amp hours, etc.) and information regarding staffing, capacities, and throughput can be empirically deduced.

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## **Endcap Design Optimization Using Mechanica**

Surety systems engineering is vital to the security of the nuclear stockpile and as a result, all components must be verified to withstand specific requirements without failure. For my project pressure is the important design requirement. Creo™ Parametric modeling software allows us to conduct various studies, such as feasibility, sensitivity, optimization, tolerance, etc. on 3-D models. Optimization studies in Mechanica allow us to analyze stress concentrations and locate any area where the yield strength may be exceeded. While there are instances where these stress concentrations are in fact negligible and can be ignored, we are searching for a more scientifically verifiable way to eliminate localized yielding. Several different techniques within Mechanica can be applied to these finite element analyses in order to create successful optimizations.

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## **Aerosol Efficiency Testing of SNM Canister Filters at Low-Flow**

A test system has been developed to measure the collection efficiency of filters which are integrated into containers storing special nuclear materials. The LANL purchase specification requires that these filters “capture greater than 99.97% of 0.45-micron mean diameter dioctyl phthalate (DOP) aerosol at the rated flow with an upstream concentration of  $65 \pm 15$  micrograms per liter.” There are two systems being built. One will be used in the TA-55 plutonium facility, while the other will remain in the RP-SVS Aerosol Engineering Facility. The TA-55 system will be used to verify operational performance without removing the filter’s canister from TA-55, and the TA-3 system will have an expanded analytical capability to help with lifetime extension efforts. The systems will allow for “in-house” testing of the filters which was not possible before. Both of these systems will have automatic data acquisition through a LabView™ software algorithm. This system is intended to be compatible with the test protocol developed by the canister manufacturer (NFT Inc., Golden CO). Preliminary tests with the first system prototype indicated two areas of discrepancy between LANL measurements and NucFilt Inc data. The first discrepancy (measured filter efficiency) has been resolved, and resolution of the second discrepancy (measured filter pressure drop) is being pursued.

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## **Is it Still Breathing? Detecting Clogged Filters on Nuclear Material Canisters**

Storage canisters for special nuclear materials have an integrated filter to allow inert gasses to enter and exit the canister while preventing the escape of nuclear material particulates. These filters can become clogged over time due to deposition of particles, or from the precipitation of solid material on the filter. Because a clogged filter could lead to a positively pressured canister, it is important to know before opening the canister whether or not the filter is clogged. LANL is designing an instrument which will make this determination, without needing to open the canister. The instrument would function by pulling a vacuum on one side of the filter, and measuring the pressure drop and mass flow rate through the filter versus time. Because a clogged filter would cause a much higher pressure drop for a given mass flow rate than an unclogged filter, the pressure drop versus flow rate can be used to determine whether or not the filter is clogged. Additionally, by measuring the total mass of air removed from the canister, the instrument will be able to determine what percentage of the canister's volume is occupied by solid material. Finally, the instrument will be able to detect whether the O-ring seal on the canister lid is leaky or secure based on whether the system is able to maintain a vacuum in the canister without constantly pumping out air. The instrument is currently in an initial prototyping phase of development. Data gathered from canister lids indicates that the methodology used in this instrumentation will be able to accurately assess the state of the filter.

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## **Weld Development for Tantalum-10% Tungsten Strength Member**

Welding of safety critical precision parts requires great attention to detail in the development of the weld. An electron beam welding process is being developed for a tantalum-10% tungsten (Ta-10W) strength member. Electron beam welding lends itself to precision applications such as this, because the beam can be shaped and focused to control power density and produce highly repeatable welds of the desired dimensions.

A preliminary process characterization was completed which consisted of linear welds along the length of a TA-10W tube. These welds covered a wide range of focus and power conditions and yielded an approximate model to predict conditions needed to achieve the specified weld depth of penetration and other desired weld shape factors. Based on the preliminary model, a design of experiments (DOEx) matrix of welds was completed, further characterizing the interaction of beam focus and power on actual strength member component circumferential welds. Further experiments were completed looking at the use of high speed beam deflection to manipulate power density for control of the weld shape, and additionally in the development of a secondary “cosmetic” weld pass for the purpose of smoothing over the previously welded joint.

Going forward, the welding beam will be evaluated to determine its size, shape, and power density. This characterization of the electron beam will be completed on both the process development welding system located at SM39 and the production welding system located at TA55. This beam characterization will assist in the transfer of the process from development to production, and additionally provide a baseline for process trouble shooting and maintenance.

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## **An Economic Case Study: Argon Systems for Glovebox Inertion**

The ability to inert gloveboxes is an essential component in the handling and manufacturing of plutonium at Los Alamos National Laboratory (LANL). The current systems in place at LANL are out of date or in need of replacement. The goal of this study was to economically compare four different methods for inerting gloveboxes; (1) inert purge with argon gas (base case), (2) a Dri-train<sup>®</sup> with argon gas (current method), (3) a nitrogen generation system with a Dri-Train<sup>®</sup> and (4) a nitrogen generation system with purge. The four methods were examined using a discounted Incremental Net Present Value (INPV), Discounted Cash Flow Rate of Return (DCFROR) and also through the use of both annual cash flow and cumulative cash flow diagrams. These methods of analysis relied on the estimation of flow rates based on inexact measurements and a preliminary design estimate for costs. The results of these analyses revealed that of the three was two potentially cost avoidance retrofit schemes within the lifetime of the project (17 years) with a goal rate of return of eight percent. The DCFROR for options 2, 3, and 4 were found to be 4.7%, -0.7% and 8.6% respectively. However, all options have the potential of saving on facility gas costs on an annual basis only option 2 and 4 are capable of reducing expenditures within the lifetime of 17 years. The recommended course of action would be to construct a lab scale process capable of executing all four system designs to experimentally determine flow rates and inerting ability of each system. It is also recommended to determine the actual lifetime of the N<sub>2</sub> generation system and identify ways to cut maintenance costs such as filter replacement opposed to the whole unit replacement costs used in this study, as these maintenance costs cuts would dramatically alter potential savings of systems 3 and 4. It is also recommended to further investigate costs using a more in depth evaluation of costs like a definitive or detailed estimate.

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## **Fluid Injector Testing and Timing Modifications**

The Fluid injector system is a design project created by students at the University of Colorado. This system dispenses 1L of stored liquid and then, after some time, dispenses an additional 0.1L of stored liquid from a separate reservoir. The aim of this study is to understand the minimum time it takes to dispense each volume of liquid and how to change the system timing so that the second liquid is dispensed immediately following the first.

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## **Surface Perturbation Theory in MCNP6 to Estimate Perturbed Eigenvalues**

Adjoint-based sensitivity theory is used to approximate  $dkeff/dr$ , the derivative of the neutron transport k-eigenvalue with respect to the location of a material interface. This study demonstrates how a change in  $keff$  can be estimated for a sphere translation and for a sphere-to-ellipsoid transformation using perturbation theory. Specifically, a surface perturbation is computed using the values of  $dkeff/dr$  on each differential surface area on an unperturbed sphere. Each differential area is then expanded or contracted mathematically in order to estimate the change in  $keff$  for a specific perturbation.

Both symmetric and asymmetric problems were tested using these methods. To do this, a Monte Carlo method previously developed in MCNP6 to estimate the change in  $keff$  due to uniform surface expansions and contractions was modified to estimate the change in  $keff$  for sphere translations and sphere-to-ellipsoid transformations. The results from the perturbation code in MCNP6 were then compared to reference results, which were found by manually computing the reference  $keff$ 's using two different MCNP6 input files. For problems where the volume of the sphere changed, the differences between the perturbation estimates and the reference results were less than 10%. For problems where the volume was conserved, the differences between the perturbation estimates and the reference results were 20% or greater.

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## **Testing the Light Ion and Delayed Gamma Capabilities in MCNP6**

The mission of the Domestic Nuclear Detection Office (DNDO) is to quickly and reliably detect unauthorized attempts to import or transport special nuclear material (SNM) for use against the United States. Developing detection equipment to meet this objective requires accurate simulation of both the detectable signature and detection mechanism. MCNP6 is capable of transporting the various types of radiation encountered in these scenarios; however, the accuracy of MCNP6 must be quantified such that we can be confident in the results of the simulations. Presented here are combinations of closed form analytic solutions and experiments for comparing the light ion library and delayed gamma simulation capability in MCNP6. The light ion capability was tested by comparing simulations of neutron emission using Sources 4C and MCNP6. The simulations used the light ion transport libraries, from TALYS-based Evaluated Nuclear Data Library (TENDL), with MCNP6. The delayed gamma capability in MCNP6 was compared to analytic closed form solutions of the emission gammas. Seven parent isotopes were used for testing. The selection criteria for the parent included: (a) the parent must decay by beta emission into a stable granddaughter; and (b) the total decay chain must possess <100 gamma emission lines. Decay times examined were 1 minute, 1 hour, 1 day, 1 year, and 100 years. Comparisons between MCNP and the closed form analytic solutions showed that for isotopes with half-lives larger than 1e10s the percent differences are large (>100%). For isotopes with half-lives less than 1e10s the percent differences are much smaller (<30%). Based on these results, changes were made to the time integration scheme in MCNP6 to correct for the larger errors.

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**LA-UR:** 13-25530

## **A Robotic System for Accurate Covercoat Application**

During covercoat application, steel tooling is used to guide a plastic covercoat onto a detonator cable. This manual process often scratches the fragile cables, which leads to a costly rejection of the part. As one part is assembled at a time, the process is also inefficient and requires a high level of manual dexterity.

This poster covers the design of a robotic system that can replace the manual process. The robotic system was designed with the following goals in mind:

- Minimal system complexity
- Primary use of off-the-shelf components
- No direct contact with the cable, in order to avoid damage
- A redundant safety system
- Low cost
- Improved process throughput

The proposed robotic system uses vacuum grippers and computer vision to achieve both high accuracy and a low rejection rate.

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## **Resistance Thermal Device Outgassing Measurements for DARHT Axis II Cathode**

In DARHT Axis II injector, the supporting components of the cathode absorb energy causing their temperature to rise, which could lead to physical changes in the position of the cathode. There is a need for dependable temperature measuring device to monitor changes while not contaminating the sensitive cathode. A Resistance Thermal Device (RTD) was selected and works by measuring the resistance change across a known metal to determine temperature. It is a simple solution to the key environmental requirements of a high vacuum system and high temperature ranges. To test the RTDs' outgassing properties a chamber with a Residual Gas Analyzer (RGA) was assembled so that temperatures could reach approximately 350°C using a vacuum compatible halogen heat lamp, while pumping down with a turbo pump to achieve 1E -7 Torr. In this system four RTD elements were tested to see what contaminants were outgassed as they were heated. This poster will present the data and results, which conclude the optimal RTD for the given environmental factors.

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## **DARHT Cold Cathode Studies and Beam Emittance** **Diagnostic Design**

The Dual Axis Radiographic Hydrodynamic Test facility (DARHT) uses two 50 m long relativistic electron beam accelerators to produce X-rays when normally incident on heavy-metal targets at the end of the beam line. The produced X-rays provide time-resolved radiographs of materials that undergoing a hydrodynamic shock. DARHT Axis-II currently utilizes a thermionic cathode to produce electrons for its radiography. The goal of this project is to aid in the design and manufacturing of a cathode test stand to study long-pulsed or multi-pulsed cold cathodes as a replacement for the current implementation on Axis-II. The study will quantify the gap closure physics of different cold cathodes, emittance, and current density distributions. A pepper pot and scintillator are being designed to optically measure the emittance of the beam and the uniformity of the current density distribution. These possible upgrades and design changes are part of an overall goal to evolve and further the design of Axis-II within the DARHT facility for greater efficiency and robustness.

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## **New Test Section for Horizontal Shock Tube**

The Extreme Fluids Team of P-23 performs experiments using a Horizontal Shock Tube (HST) to study turbulence and shock-driven mixing. The test section of the HST is where the shock-driven flow is visualized using laser diagnostics and cameras. The current test section was optimized for shock-driven mixing experiments, but the HST has recently been reconfigured to study shock-driven multiphase flows, or flows with solid or liquid particles floating in a gaseous carrier phase. Because of this change in the experimental mission of the HST, there are new requirements for the test section, and we have designed a new test section to meet both technical and safety requirements. The previous test section contained several large windows to optimize viewing access, but the high pressures in the shock tube weakened it over time. The new requirements for the multiphase flow experiments allow us to reduce the glass viewport area, increasing the safety margins on the test section. The system requires that it be able to withstand the dynamic pressures from the shock wave while allowing easy access into the test section for both cleaning and the alignment of lasers or cameras. Pressure transducers, used to trigger the cameras and lasers, are installed on the test section to provide accurate triggering. Our new design ensures that we meet these requirements, and that the new test section mounts with the existing shock tube.

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## **Improvements in MCNP6 Cosmic and Terrestrial Background Particle Fluxes**

There are many reasons to be interested in the amount of background radiation on the surface of the earth, including nuclear materials detection. This background radiation is the combined result of cosmic radiation and radiation caused by naturally occurring materials in the soil. When cosmic particles, specifically protons and alphas of sufficient energy, enter the atmosphere they collide with atmospheric particles initiating a cascade of additional particles. The particles that reach the earth's surface contribute to background radiation. This process can be simulated using Monte Carlo methods and a model of the atmosphere that provides values for conditions at different atmospheric levels, above specified geographical grid points. Relevant conditions include the temperature, atmospheric pressure, and molecular composition of the air at various altitudes. By utilizing this model, the surface background radiation levels produced by terrestrial and cosmic sources can be calculated. Los Alamos National Laboratory will incorporate this background data into its MCNP6 particle transport software. Current research and efforts are being made to improve the accuracy and abundance of the data to be included in the software.

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## **Testing, Adjusting and Balancing Facility HVAC Systems**

Heating, Ventilation and Air Conditioning (HVAC) systems are designed to maintain air quality and occupant comfort. HVAC systems are one of the largest energy consumers in office buildings. It is important to keep these systems operating as efficiently as possible. HVAC system design and operation must follow all local and state building codes, while meeting compliance with federal energy efficiency standards.

To test, adjust, and balance the air distribution for an HVAC system various instruments are used to measure airflow, water flow, static pressure, velocity pressure, temperature and relative humidity. Some of the instruments used are the Pitot tube, manometer, pressure gauge, anemometer, flow-measuring hood, Venturi tube, thermometers, and psychrometers. In this study we decided to concentrate on two different buildings with similar floor plans. These buildings constructed in the 1970s have had modifications to the HVAC systems to optimize efficiency and are now in the process of being re-commissioned.

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## **Material Transport Cart Development and Testing**

Technical area 55 (TA 55) work encompasses a variety of tasks including transportation of fissionable materials using material transport carts. These carts must meet criticality specifications along with safety guidelines as set by the DOE. Two shelved carts have been utilized for 30 years to move materials; these carts allowed the workers to safely transport up to six canisters simultaneously. In October 2012, DOE Order 420.1C Chapter III set a new cart criterion stating that the canisters must stay in place during a natural disaster. The criterion was met by weighing down the carts and implementing two canister slots for each shelf. An ergonomic evaluation utilizing the Ohio Bureau of workers compensation threshold lifting guidelines (OHBWC –TLV) determined that lifting from the bottom shelf placed the workers at an extremely high risk of back injury. With 80% of Americans complaining of back pain, and with the lab having 143 injuries from lifting in the last 5 years, management deemed this risk unacceptable. Being allowed to only use the top shelf forced the workers to transport two canisters at a time, reducing productivity and increasing the time required to transport materials. An engineering solution that met ergonomic and worker needs had to be developed. A new cart was designed using anthropometric data, the OHBWC-TLV, the NIOSH lifting guide, and the DOE order. The cart is on its second prototype, redesigned to better fit worker needs. This cart allows transportation of four canisters while staying at an anthropometric height and a maneuverable weight. Workers can reach all four slots while maintaining a low risk to back injury. A survey was developed and implemented to gather worker feedback. Further prototype improvements are being developed from their input. Implementation of the ergonomically designed cart should lead to a safer and more efficient work environment.

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## **An Introduction to Nuclear Criticality Safety**

Fissile material, mainly uranium and plutonium, is an integral part of the nation's interests in national security, energy, and technology. The Nuclear Criticality Safety group here at LANL is responsible for providing the technical guidance for the design of equipment and processes and for the development of operating procedures that helps ensure a criticality accident does not occur during the handling and processing of fissile materials. In light of this, a thorough knowledge of both the physics governing the phenomena of nuclear criticality and formality of operations is vital in order to be a successful criticality safety engineer. Since the production of fissile material during World War II, sixty known criticality accidents have occurred resulting in twenty-one deaths. At the end of the day, criticality safety is about keeping people safe. A criticality accident not only immediately produces a potentially lethal environment for personnel, but also releases hazardous material that may contaminate the surrounding area. The nuclear criticality safety discipline provides technical expertise to facility management, operations personnel, and other safety disciplines to help ensure these radiological consequences do not take place. The only way to absolutely guarantee no hazard with fissile materials is to conduct no operations with the material at all. However, because of the importance of these materials, operations must be conducted and done so in a safe manner by utilizing basic laws of neutron physics, principles of safety engineering, and operational management practices.

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## **Ensuring Health & Safety During a Process Change**

The purpose of this research project was to document the current state of Occupation Medicine's (Occ-Med) ability to provide excellent, supportive Health & Safety services, specifically with regards to the Code of Federal Regulations (CFR) 851 compliance, for each fundamental business and mission activity at Los Alamos National Laboratory (LANL). To accomplish this task, interviews were conducted with all relevant medical program surveillance owners and workers. These details were converted into individual flow diagrams containing current communications practices, specialized directives, and specifics related to enrollment, monitoring, and disenrollment for medical surveillance and certification compliance. Additional information on enrollment numbers per program, frequency of individual and system reviews, and a gap analysis was conducted to investigate areas of incongruence. On the macro level, the goal is to generate discussions on the role Occ-Med plays in ensuring LANL's compliance to CFR and other regulatory rules. This includes all personnel directly and indirectly connected to Occ-Med and the LANL facility, as well as the community-at-large. For the micro level, the aim of the project is to issue a centralized and streamlined process flow that prevents the possibility of individual or section failures from occurring. This endeavor is being completed during a conversion from traditional medical records and various manual, labor-intensive surveillance efforts to an automated, system-wide, electronic format—Occupational Health Manager (OHM). The need for ensuring Health & Safety compliances are met is critical. Therefore, documentation of existing surveillance processes, gap analysis, and the construction of a centralized surveillance/certification process is the path to successful implementation of the electronic medical record.

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## **Gait Analysis While Wearing PPE Booties in Two Different Conditions**

At Technical Area 55, workers wear personal protective equipment (PPE) booties in the Plutonium Facility (PF-4) to reduce the risk of spreading contamination throughout the facility. PF-4 workers use approximately 4000 pairs of booties per month and the current booties have been used for the last 20 years. Booties may have the potential to increase muscular stress and the risk of slipping. There are dozens of different types of manufactured booties currently on the market. The objective of this project was to establish if PPE booties affect the normal gait cycle under two different conditions (clean and dusty floor surfaces) and verify which bootie has the least affect on gait. The goal is to determine the most appropriate PPE bootie which would mitigate worker's risk of injury and slipping.

Testing was conducted on the six different types of booties with two different conditions at the University of New Mexico Center for Gait and Motion Analysis. The data was collected through the use of Vicon infrared cameras, Vicon collection software, and AMTI force plates. The analysis examined complete gait cycles to determine how the different types of booties affected gait when compared to normal gait without booties. The parameters of this analysis included cadence, velocity, step and stride length, step and stride time, step width, ratio of single to double limb support, and the joint forces. The results of the analysis provided a greater understanding on how PPE booties affect the operators.

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## **SB-TS – Quality Review of Proposed Document Safety Analysis and Records Management**

The Department of Energy Nuclear Safety Management Rule (10CFR830) lays out the regulations for non-reactor nuclear facilities to operate, such as are found at the Laboratory. The Rule is divided into two Parts: Subpart A Quality Assurance Requirements and Subpart B Safety Basis Requirements. Both Parts of the Rule are important for the operation of nuclear facilities at the Laboratory. The quality of safety basis documents for nuclear facility operations is extremely critical with the Laboratory under constant scrutiny on the ability to deliver safety basis documents of high quality to the DOE Field Office for DOE's subsequent approval. In addition, document control and records management of safety basis documents, including supporting documentation, is subject to Subpart A of the Rule.

To support Subpart A requirements of the Rule, the following work was completed: A review of a Preliminary Documented Safety Analysis for the new transuranic (TRU) waste facility at LANL was undertaken. The review is part of a Quality Review Board within the Safety Basis Division, established to ensure the technical quality of safety basis documents before their submittal to DOE.

Also, Records Management has been updated to a more advanced standard. The updated system is available via an online server that will be more readily available than the previous.

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## **Radiological Release Dispersion: The Potential Effects of Wind Currents**

A radiological release dispersion model has a primary goal to calculate the dose consequence distribution emitted from a plume generated by a spill, fire, or detonation event. One parameter in the model analyzes the effect of wind currents at the site boundaries and in the surrounding areas of Los Alamos, New Mexico. Wind currents were measured by four LANL towers (12 m) located in: TA-6, TA-49, TA-53, and TA-54. Data for direction, velocity, stability, and precipitation were recorded by each tower per hour for years 2003-2012, excluding 2009. The removal of year 2009 from the data set is attributed to TA-6's tower having mechanical malfunction with its anemometers for two months. The provided years and towers were used to create wind roses describing both wind velocity and stability annually. Wind roses were also made for ranges 2003-2007 and 2007-2012 to serve as visuals for possibility of quantitative alteration. The results conclude the frequency and variability of wind velocity and stability from 16 directions (22.5° sectors). Supplementary wind roses for the respected towers and years were also created using the U.S. Naval Observatory's definition of daylight to display comparison between day and night. Additional towers near and within canyons were also monitored to observe possible channeling effects. Channeling has the potential to alter the original path of a plume.

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## **Health and Safety Analysis of the Waste Treatment Facility**

The Radioactive Liquid Waste Treatment Facility at Los Alamos National Laboratory was constructed in 1962, long before ergonomics became a safety concern. Many of the valves and other controls that must be managed every day are located in such a way as only a thin person over six feet tall could operate them with reasonable safety. However, most workers do not have those physical attributes. Some controls are located behind pipes, so workers must maneuver and extend their bodies in awkward positions to accomplish their work. As a result, they must stretch and contort themselves, risk falling, etc., and risk breaking a piece of equipment. The design of the workspace increases the risk of injuries because it was not designed with ergonomics in mind which may lead to a decreased quality of life due to injury. Previous analyses have been conducted with few changes taking place. During the summer of 2013, a new analysis was conducted. Suggestions will be made for each of the identified safety concerns.

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## **Establishing The Radiation Protection Database**

Over the last 70 years, radiation protection has been an integral part of Los Alamos National Laboratory's (LANL) safety initiative. The radiation protection program exists to ensure that radiological work is performed safely while maintaining employee exposure as low as reasonable achievable (ALARA). Using external dosimetry, LANL monitors and regulates the radiation exposure of its employees in the workplace. Over the past several years, the External Dosimetry Team created a database of historic radiation protection information to ensure accurate exposure monitoring and surveillance across LANL.

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## **Rotator Cuff Strength Balance in Glovebox Workers**

Los Alamos National Laboratory (LANL) relies heavily upon the use of shielded gloveboxes (GB) for the performance of a vast number of tasks. LANL currently maintains more than 700 operable gloveboxes, the majority of which are located at the Plutonium Facility (TA-55). Glovebox work typically involves a significant amount of shoulder rotation (e.g., transferring items into and out of airlocks, passing items down the length of a GB, etc.). Shoulder rotation puts a great amount of stress on 4 intrinsic shoulder muscles collectively referred to as the rotator cuff. This study investigated the strength ratio of the shoulder rotator cuff muscles in GB workers at TA-55 and compared this ratio to established healthy norms. Handheld dynamometry was used to quantify force produced in the motions of shoulder internal and external rotation. The results demonstrated an overall deficiency in GB worker external rotator strength, which demonstrates the need for the implementation of various designed engineering solutions to reduce stress on the rotator cuff musculature. Collaboration between the ergonomics team and management will allow for the institution of controls that will improve worker safety, comfort, and productivity.

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## **Chemical Inventory and Safety**

LANL employees in the Logistics division work with over 600 chemical products that require precautionary handling processes. Because the material safety data sheets (MSDS) are stored in a range of locations, some precautionary health information may not be readily available in the case of an accident or for work planning. Thus, in order to maintain an incident-free workplace, workers must have access to a lab-wide database of the products used. This project aims to improve worker safety by using MSDSonline to make chemical safety information more accessible to employees. The project supports the safety of Logistics/MSS by reviewing current MSDS, revising ChemLog inventories, and entering findings in MSDSonline, a commercial database. Students research toxicological effects of long-term exposure to chemicals and any established OSHA regulations and consensus standards for specific reagents. The health effects of each chemical are studied to ensure that workers wear adequate personal protective equipment. Additionally, each entry provides an executive summary of the immediate hazards and emergency procedures for each chemical. The project will help employees develop a working knowledge of chemical products utilized in the performance of maintenance for the Los Alamos National Lab. They will include procurement, inventory, safe use practices, storage and eventual disposal per State and Federal regulations. MSDSonline eBinder is an easy way for employees to access safety information and precautions about chemical products before they use them. The eBinder can be used to promote workplace safety by increasing worker knowledge of potentially hazardous chemicals. By making employees aware of the possible health hazards each product may have, we are making the work place a safer and healthier place. We are striving to make this process efficient and utilized by all employees here at Los Alamos National Lab.

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## **Automating the Green is Clean Waste Process**

The legacy database system used to manage this waste is being replaced by the new Waste Compliance and Tracking System (WCATS). I have been assigned to help automate the Green is Clean(GIC) waste processing, this is done through learning the processes used with GIC waste in order to provide the correct workflow for the end user within WCATS through interviews with GIC waste handlers. I have asked them what they would like to see better in the process or things that could be improved. I will be providing a way to test the functionality of the work flow for GIC waste within WCATS so that the end user will be able to test and see what other improvements they would like to see in the process. I will also write a requirements document to specify what the system is required to track for the GIC waste disposal process.

There will be many improvements to the work process. Moving to WCATS will help the Waste Management Coordinator have less work with entering in all of the waste Items, as they can be entered in to the system by the waste Generator at the Generation site of the GIC waste. It will allow more Reports to be outputted for use by the end user, which will be used for reporting on GIC waste generation throughout the Laboratory. The use of mobile devices for the system will allow work to be done out in the field removing the need for paper log sheets to write down all of the waste item information. The use of mobile devices will allow the waste to be tracked in the system from the characterization of the waste until it is disposed of properly.

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## **Reason Software**

This report examines the REASON software. REASON is a software used to examine root cause analysis and contains a rule based expert system. Utilization of REASON begins by asking the user to enter a problem statement then leads the user to identify step by step why each part of the problem occurred. By the entered information REASON is able to ask more increasingly detailed questions. When finished eventually a TREE model will be created with an automatic narrative and analysis as well as graphics and other report elements. Typically REASON is used in quality improvement, safety and health, medical information systems, maintenance and reliability efforts. As a 32bit Windows application it can run on standalone or Windows server. The application runs on all Windows versions, requires 100mb of disk space. REASON includes a LL broadcasting system and a CAT e-mail reminder service and all cases are stored in the MS SQL REASON repository. The repository manager allows the network administrator to manage the repository.

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## **Automating the RFI Process with SharePoint**

At LANL, all formal engineering design changes are initiated using the Conduct of Engineering procedure AP-341-517, Design Change Form. One part of the procedure is the Request for Information (RFI) process. The RFI process is a mechanism that allows project participants such as engineers, subcontractors, construction superintendents and procurement officers to submit a formal question to Project Engineers (PE). PEs can then send the RFI to be responded to by an appropriate expert on the subject matter, or respond to the RFI themselves. When the RFI is returned, the PE and any applicable authorities must approve the response and sign the RFI. From there, if the RFI requires a design change, further documentation is developed, using the RFI as a basis for the change.

Currently, LANL procedure requires the use of a word document to generate the original RFI, then attaching the document to a series of emails. For approval, RFIs are then printed out and hand carried to the various authorities for signature. RFIs are tracked on a project-by-project basis, with little to no consistency from one project to the next. Some use an Excel spreadsheet, hand populated by a dedicated RFI tracker. The spreadsheet stores the dates of each step in the process, from initiation to closing, as well as notes concerning the RFI and the status of any further documents.

The intent of the SharePoint RFI (SPRFI) Process is to automate the RFI process, such that hard copy processing is eliminated. The paperless SRFI process completely eliminates the need for hand processing, greatly increasing operational efficiency of the entire Design Change process. Integration with an already in-place SharePoint Design Change (DCF) system provides users with a one stop shop for all necessary elements of design changes and relevant project information.

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## **Semi-Automated Welding**

Semi-automated and fully automatic welding systems are welding processes that are mostly computer controlled. Welding is accomplished by automating the torch or part motion and using an electronic controller to recall a set of welding parameters. This allows improved weld quality and repeatability. Eliminating the human factor as much as possible reduces the possibility of human error and increases output. Using semi-automatic and fully automatic welding systems can have other benefits. For example slides, mechanical fixtures, and welding torch can be installed into a glove box or welding chamber and be controlled by the electronic controller to perform the welding operations. Performing welds inside a glove box or welding chamber is useful when hermetically sealing a hazardous material in a container; it also does not allow the weld operator to be exposed to any hazardous welding fumes. Welding in an inert atmosphere glove box or welding chamber also allows for better control of the welding process by eliminating unwanted atmospheric gases such as oxygen, nitrogen, and water vapor that can reduce the quality of the weld or make the welding more difficult. It has been determined that using semi-automated and fully automatic welding systems within TA-55 facilities has provided a safer work environment and increased production and quality of our product, thereby allowing us to meet our milestones and mission. As a student I will be assigned to work with a mentor/SME to learn to safely operate equipment and to develop of weld schedules.

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## **Characterization of Ferritic Steels for Nuclear Applications**

Ferritic steels are attractive materials for core applications and pressure vessels in Generation IV reactors because of their high thermal conductivity, good corrosion resistance and low void swelling. In developing these materials, it is important to understand mechanical properties like tensile behavior, fracture toughness and creep behavior and its relation to the microstructure since the properties are led by microstructure and processing. Thus, it is crucial to understand the initial microstructure and processing routes for candidate materials. In this research, initial microstructure and mechanical properties of high Cr F/M steels HT-9, MA-956 and Kanthal AF having different processing routes are investigated. In HT-9,  $\delta$ -ferrite formed during processing and alpha prime (formed during irradiation) can strongly affect the mechanical properties. The  $\delta$ -ferrite amount was analyzed in two different heats of HT-9 with slightly different processing routes and an increased Cr content was observed in  $\delta$ -ferrite compared to  $\alpha$ -ferrite. In order to quantify hardening observed related to  $\alpha'$  formation, HT-9 steels were shocked at a peak pressure of 11 GPa and subsequently annealed at 380°C and 440°C for 18 months. Nanohardness results suggest that an increased density of  $\alpha'$  causes a larger increase in the hardness at 380°C than at 440°C. Attempts were made to produce thin walled tubing in MA-956 ODS steels and Kanthal AF starting from solid bar or plate material. Cracking was observed in MA-956 related to the initial large grain size (larger than 1 mm) while Kanthal AF was successfully drawn to thin walled tubes starting with a much smaller grain size (less than 30 microns).

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## **Effects of Temperature on Homogeneity of Phospholipid Bilayers**

Controlling cell growth on different surfaces is crucial for many applications. For instance, cell lines benefit from the use of positively charged polymers, which enhance their ability to attach to culture plates. Previous studies of lipid bilayers deposited on a polyelectrolyte multilayer show that the size of the water gap between the lipid bilayer and the polyelectrolyte substrate can be influenced by environmental conditions - and a “floating bilayer” can be created.

In order to verify whether lipid bilayers are able to maintain stability and thus sustain cell life at culture conditions, lipid bilayers on various supports were examined over time in different parameters, utilizing fluorescence microscopy to investigate their homogeneity and durability. Essentially, temperature affects the molecules of the lipid bilayer; their fluidity, permeability, and hence the ability of cells to survive are all altered.

It could be shown that lipid bilayers deposited on polymeric cushions tended to be more stable in different parameters than those without the polymer support. In conclusion, the lipid bilayers were able to maintain stability at cell culture conditions - especially if they were deposited on top of said polymeric cushion. Thus, cells could potentially be grown on such bilayers, allowing for discovery of more applications and further growth in investigating cell culture and its possible uses.

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**LA-UR:** 13-25730

## **Programming and Machining of Several Common Logos Using the CNC Mill**

Machining is more technically complicated than one would think. There are many measurements, calculations and programming involved prior to cutting into the material. Through this machining exercise we discovered in order to be a skilled machinist a strong mathematics background is needed. To demonstrate our machining ability, six interesting logos were machined out of a block of aluminum. The following steps were performed:

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3. The origin points were then determined on the block of aluminum to initiate milling the logos
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6. An ellipse cut was first made by finding the radius of the electron paths using a radius gauge to find the arc
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9. The radius of the circle from the center point was located in order to mill the nucleus and the three locations for the electrons
10. Once all the measurements were located a milling program was program designed to mill the atom logo

**Name:** Ethan Cheng  
**Program:** UGS  
**School:** Rutgers University  
**Group:** MPA-CINT  
**Mentor:** Aditya Mohite  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25462

## **Stacking Individual Sheets of Two-Dimensional Materials for Next Generation Optoelectronics**

To produce graphene and other atomically-thin mono-layered nanomaterials, the traditional method is to mechanically exfoliate the layers by applying scotch tape to both sides of a crystal and peeling it apart. This method produces flakes that are single-layered and extremely high in quality; however, the yield is extremely low. Because of this, novel multilayered devices are often fabricated with flakes made by chemical exfoliation, which has a high yield of flakes but of inferior quality. In order to improve and characterize the true properties of such devices, a method has to be created in which mechanically exfoliated flakes can be identified, isolated and deposited on other flakes. The development of this method using common laboratory equipments would exponentially facilitate access to high-quality novel multilayered devices, which cannot be achieved otherwise. Having the capability to overcome fabrication limitations of using high-quality mechanically exfoliated nanomaterials has potential of making significant contributions to the fields of electronics, optoelectronics, and energy harvesting.

**Name:** Eric Davis  
**Program:** UGS  
**School:** Texas Christian University  
**Group:** MPA-11  
**Mentor:** Pantea Cristian  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25467

## **Resonance Ultrasound Spectroscopy Measurements of Sandstone**

Deep underground wells, such as those of interest to the oil and gas as well as geothermal industries, are often found in large sandstone formations. In order for drilling, enhancement, and advanced engineering techniques such as hydraulic fracturing (fracking) to be efficient and successful, the mechanical properties of materials that make up the reservoir must be accurately determined. Resonant Ultrasound Spectroscopy (RUS) is a powerful, nondestructive technique that can be used over a wide range of temperatures and on small samples (on the order of millimeters) to determine a material's physical properties such as elastic moduli. RUS's high sensitivity determines these material properties with extremely high accuracy from the natural mechanical resonances of a sample that depend upon certain physical properties and a specific geometry. A swept frequency acoustic signal is applied to the sample via one transducer while another transducer records the mechanical response of the sample in order to identify the resonance frequencies. In contrast to single crystals or high quality polycrystalline samples typically probed by RUS, the porous and attenuating nature of sandstone makes an acoustic study of sandstone very challenging. In addition, the sandstones must be studied at high temperatures in order to simulate conditions that would be found in the field. We will present our work on the temperature dependence of the elastic moduli of sandstone (between room temperature and about 205 °C), as well as our experimental setup (computer-controlled Labview program) and other supporting work. It was found that Berea sandstone is a very soft material, with a bulk modulus of about 6 GPa (e.g. the value for Aluminum is 76 GPa). Additionally a softening (about 10%) with temperature decrease was determined, down to a temperature of 110 °C, followed by a hardening down to room temperature (~ 7%).

**Name:** Vaughn Hartung  
**Program:** GRA  
**School:** University of Oregon  
**Group:** MST-7  
**Mentor:** Dominic Peterson  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25180

## **Characterization of Sylgard®184 and 186 Silicone Elastomer Formulations**

A material under the trade name Dow Corning® Sylgard®, is an elastomeric silicone used in a variety of industrial applications due to its inexpensive manufacturing cost, thermal and chemical stability, and general resistance to harsh environments. A vast selection of silicone formulations exist and each material recipe exhibits unique material properties. In order to provide a rationale for selection from the variety of silicone formulations available, the rheological, mechanical, and thermal properties of Sylgard®184 and Sylgard®186 formulations have been examined and compared for recommendation.

**Name:** Alicia Herrera  
**Program:** UGS  
**School:** University of California- Davis  
**Group:** MST-8  
**Mentor:** Ellen Cerreta  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-24783

## **The Role of Interfaces on Shock-Induced Damage in Two-Phase Metals: Copper-Lead**

For ductile metals, dynamic fracture during shock loading is thought to occur through void nucleation, growth, and then coalescence, that eventually leads to material failure. Particularly for high purity metals, it has been observed by numerous investigators that under incipient spall conditions, voids appear to deterministically nucleate at some grain boundaries, but not others. However, for materials of engineering significance, those with inclusions, second phase particles, or chemical banding, the role of grain boundaries versus other types of interfaces in damage nucleation is not well understood. To approach this problem two materials have been systematically investigated: (1) high purity copper, and (2) copper with 1 wt-% lead. The behavior of lead precipitates at copper grain boundaries on damage nucleation and evolution will be investigated using shock loading and release experiments.

**Name:** Jane Heyes  
**Program:** GRA  
**School:** Stanford University  
**Group:** MPA-CINT  
**Mentor:** Hou-Tong Chen  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25729

## **Hybrid Cut-Wire Metamaterials for Broadband Terahertz Modulation**

Metamaterials are structures designed on a subwavelength scale to influence electromagnetic waves. They allow for a variety of unique phenomena not seen in natural materials, a boon for the terahertz (THz) regime. Waves with THz frequencies have few naturally occurring materials suitable for device design, making metamaterial-based structures important for using this part of the electromagnetic spectrum between electronics and infrared (IR) optics. In this project, we design a series of metamaterials consisting of gold cut-wire arrays integrated with silicon at critical regions. Below the resonance frequency the metamaterials allow for high transmission. However, when the silicon is excited by an IR pump and becomes conducting, the cut-wires behave like a metal wire grating, blocking the incident THz waves polarized along the wires. In such a way, we accomplish broadband modulation of THz waves with relatively low pump power of the IR laser as compared to a plain silicon-on-sapphire. We fabricated the metamaterial samples using photolithography methods, metal deposition, lift-off, and reactive ion etching using facilities in the CINT clean room. The samples were characterized using an optical-pump THz-probe spectrometer. The experimental results are in excellent agreement with the full-wave numerical simulations.

**Name:** Benjamin Hollowell  
**Program:** UGS  
**School:** University of New Mexico- Los Alamos  
**Group:** WX-9  
**Mentor:** Dana Dattelbaum  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-21143

## **Shock Initiation of the TATB-Based Explosive PBX 9502 Cooled to 77 Kelvin**

Recently we reported on shock initiation of PBX 9502 (95 wt.% tri-amino-trinitrobenzene, 5 wt.% Kel-F 800 binder) cooled to -55OC or 218K (J. Appl. Phys., 112, 74909 (2012)). Shock waves were generated by gas-gun driven plate impacts and reactive flow in the cooled PBX 9502 was measured with embedded electromagnetic gauges. Here we describe methods to cool the explosive below -55 C; down to liquid nitrogen temperature of -196OC or 77K. As described in the reference above, we start cooling the PBX 9502 by flowing chilled nitrogen (N<sub>2</sub>) gas through channels in an aluminum plate on which the sample is mounted and through a coil surrounding the sample. Temperature in the sample is monitored using type-E thermocouples, and samples are cooled slowly at ~ 1-3OC/min. Cooling rate is controlled by re-warming the chilled N<sub>2</sub> gas using in-line heaters. After minimum temperature is reached using chilled N<sub>2</sub> gas, we flow liquid nitrogen (LN<sub>2</sub>) through the channels in the sample mounting plate and coil. In this way, minimum temperatures of 77K are reached. Preliminary results show continued reductions in temperature cause continued reductions in shock sensitivity. For example, consider the following three experiments with approximately equal inputs produced by impacting the PBX 9502 with Kel-F 81 flyers traveling ~ 3.23 km/s. The sample temperature was systematically varied and, as a response, the distance to detonation (XD) was measured. At 23OC, XD = 3.2 mm, at -55OC, XD = 3.9 mm and at -196OC or 77K, XD = 6.4 mm. Larger XD equates with reduced shock sensitivity. Hence, reducing the temperature below -55OC further reduces the sensitivity. Wave profiles were also obtained during the shock to-detonation transition and will be presented.

**Name:** Terri Lin  
**Program:** GRA  
**School:** University of Oregon  
**Group:** MST-7  
**Mentor:** Dominic Peterson  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25503

## **Development of Polyaniline Conductive Coating**

Polyaniline (PANI) is considered as one of the most promising electrically conducting polymers due to its low density, high environmental stability, moderate conductivity and inexpensive polymerization. However, PANI's poor solubility limits its performance. It is not soluble in conventional organic solvents, rather in solutions such as N-methyl-2-pyrrolidinone (NMP). Though PANI is soluble in solvents such as NMP and m-cresol, these solvents are hard to remove during processing. As conductive coatings and resins gain interest, being able to dope polyaniline in water and organic solvents would be beneficial to help suspend polyaniline particles in resins quickly and easily. Polyaniline was doped in water and organic solvents, methanol and THF to create a conductive coating with an acrylate resin. The protonation process of PANI was achieved by immersing the polymer into solutions of acid. Four acids, 2-acrylamido-2-methylpropane sulfonic acid (AMPSA), camphorsulfonic acid (CSA), dodecylbenzene sulfonic acid (DBS), citric acid (CA) were used in this experiment. X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) and UV-Vis Spectroscopy have been used to indicate the degree of crystallinity and polymer conformation. Studies have shown that methanol results stronger polymer-solvent and hydrogen bonding interaction, which favors the expanded coil conformation and allows dopants to attack the protonation sites more easily and is therefore a better solvent. PANI doped with AMPSA, CSA, and DBS is more crystalline due to sulfonic acid's enhancement on solubility of PANI. However, DBS, CSA and CA-doped PANI have higher conductivity compared to AMPSA doped PANI since the polymer is only partly protonated due to its additional interactions with the acid.

**Name:** Analisa Martinez  
**Program:** UGS  
**School:** University of New Mexico  
**Group:** NCO-2  
**Mentor:** Brenda Griego  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25730

## **Programming and Machining of Several Common Logos Using the CNC Mill**

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19. The radius of the circle from the center point was located in order to mill the nucleus and the three locations for the electrons
20. Once all the measurements were located a milling program was designed to mill the atom logo

**Name:** Nicholas Orenstein  
**Program:** GRA  
**School:** University of Southern California  
**Group:** MET-2  
**Mentor:** Tom Jachimowski  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25595

### **3D Flow and Temperature Analysis of Filling a Plutonium Mold**

The plutonium foundry at Los Alamos National Laboratory casts products for various special nuclear applications. However, plutonium's radioactivity, material properties, and security constraints complicate the ability to perform experimental analysis of mold behavior. The Manufacturing Engineering and Technologies (MET-2) group previously developed a graphite mold to vacuum cast small plutonium disks to be used by the Department of Homeland Security as point sources for radiation sensor testing. Models using Flow-3D computational fluid dynamics software are employed here to determine liquid Pu flow paths, optimal pour regimes, temperature changes, and pressure variations. A two-stage pouring basin consisting of a funnel and an angled cavity directs the liquid into a vertical runner. A stack of ten disk castings connect to the runner by horizontal gates. Volumetric flow rates were implemented to limit overflow into the funnel and minimize foundry returns. Simulations show that the flow follows a three-dimensional path which includes cascading over the angled ledge and non-uniform cavity filling. The mold fills upwards with two to three disks receiving metal flow in a staggered sequence. Pressure builds up in the well, where impurities were found to settle in the actual mold. Simulation results showed negligible temperature change at casting temperatures of 850 °C molten plutonium and 500 °C graphite mold over a ten second timescale. In real castings, cooling requires approximately ten minutes, so temperature effects in such a superheated scenario are unlikely to affect solidification.

**Name:** Patrick Phelps  
**Program:** UGS  
**School:** University of Tulsa  
**Group:** T-1  
**Mentor:** Scott Crockett  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25521

## **An Improved Sesame Equation of State for Argon**

Los Alamos National Laboratory has been making and storing many high quality equations of state (EOS) for a long time, storing them in the Sesame library. These are tabular libraries that contain Helmholtz Free Energy, Internal Free Energy, and Pressure as functions of density and temperature. This EOS's density and temperature ranges are 0g/cc to 28000g/ and 0K to 1.1604e8K. The original Sesame EOS for Argon comes from the 1980s, and recent Density Functional Theory (DFT) calculations as well as Quantum Molecular Dynamics (QMD) calculations suggest that the old EOS is too stiff in the upper densities. Recently, Sandia National Laboratory (SNL) came out with a new Sesame-type EOS to try to amend these errors. After a comparison, more tweaking was necessary. The new Sesame-type EOS for Argon is created here by keeping the thermal nuclear and electronic contributions from the original LANL EOS and then modifying the cold curve to account for new DFT calculations. This is being evaluated against the original EOS, the SNL EOS, gaseous/liquid/solid isothermal data, Diamond Anvil Cell data, and hughoniot shock data.

**Name:** Deesha Shah  
**Program:** UGS  
**School:** University of Illinois Urbana- Champaign  
**Group:** MPA-CINT  
**Mentor:** Abul Azad  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25732

## **Terahertz Characterization of Dinitrobenzene for Metamaterial Based Sensors**

There has been an increased interest in terahertz time-domain spectroscopy (THz-TDS) for the detection of explosives since common explosive materials have unique spectral signatures between 0.1-5.0 THz. 1,4 dinitrobenzene (DNB) and 1,3 DNB exhibit properties that are similar to explosive substances. While 1,4 DNB shares a resemblance to trinitrotoluene (TNT), 1,3 DNB is a synthetic chemical commonly used in explosive devices. Increasing the sensitivity of the sensors has always been a great challenge, particularly for thin film detection. Recently, metamaterial based terahertz sensors have shown great promise in thin film sensing via introducing strong coupling between the metamaterial and the analyte resonances. However, such sensitive detection requires spectral overlapping between the metamaterial and the analyte resonances. Therefore, it is important to characterize the analyte's properties prior to the metamaterial design. In this work, we measure the optical properties of 1,4 DNB and 1,3 DNB using THz - TDS. The measurements are collected for a 0.88 mm thick 1,4 DNB sample and a 1.5 mm thick 1,3 DNB sample in the frequency range of 0.2 to 2.2 THz. One resonance is observed for 1,4 DNB, while 1,3 DNB shows three resonances, with a constant refractive index. Metamaterials that match the resonances of these chemicals are designed for implementation in a chemical sensor.

**Name:** Katey Thomas  
**Program:** UGS  
**School:** New Mexico Tech  
**Group:** Individual Poster Presentation  
**Mentor:** Rick Gustavsen  
**Category:** Materials Science  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25544

## **Window Correction of Kel-F 800**

We propose to characterize the plastic/polymer Kel-F 800 (poly(chlorotrifluoroethylene-co-vinylidene fluoride)) for use as a velocimetry “window” in shock physics experiments. The requirement is to measure a “window correction factor.” The experimental method of Jones et al. (JAP, 88, 5671 (2000)) will be used, in which a series of experiments of the following type will be performed. An impactor disk of Kel-F 800 will be mounted in a projectile, launched in a gas gun, and will impact a sample of Kel-F 800. The velocity at impact time will be measured precisely. Because of symmetry, the true velocity at the impact interface must be  $\frac{1}{2}$  the impact velocity. The “apparent” particle velocity at the impact interface will be measured using Velocity Interferometer System for Any Reflector (VISAR, 532 nm light) and/or Photonic Doppler Velocimetry (PDV, 1550 nm light). The window correction factor is the apparent velocity divided by the true velocity. Correction factors from experiments with several projectile impact velocities will be measured. Additional information that can be obtained from these experiments is shock velocity vs. particle velocity Hugoniot points and refractive index as a function of density.

**Name:** Joshua Dolin  
**Program:** UGS  
**School:** University of New Mexico  
**Group:** CGA-CO  
**Mentor:** Steve Sandoval  
**Category:** Non-Technical  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25562

## **Feeding the Information Pipe: Communicating for a Multidisciplinary Organization**

Communication is a vital resource in every business organization, and Los Alamos National Laboratory is no different. Internal communication keeps employees informed and knowledgeable about the company they work for, and external communication maintains a strong public image for the company itself. With the new rise in technology however, communication is becoming even more important and the tools used to communicate are rapidly changing. In my poster presentation I will discuss my work this summer in LANL's communication office. I will show examples of multiple platforms used for internal communication such as LANL Today and LANL Inside, as well as external communication. The external communication includes the use of social media, news releases, and media tours. It is important to understand how to communicate in order to create a strong and unified work force, like we have here at Los Alamos National Laboratory.

This summer at the lab I worked on different projects that were strategically planned to communicate to audiences on all levels. Externally I created and managed posts on social media sites such as Facebook and Twitter, which allow the lab to disseminate information to the public, especially younger demographics. Internally I attended meetings and traveled all over the property to interview professionals and draft news briefs about their work.

Now, more than ever, it is very important to have a great public image and relationship with stakeholders. My summer at LANL was spent drafting projects and communicating to important people both inside and outside the laboratory.

**Name:** Jesse Giron  
**Program:** UGS  
**School:** University of New Mexico  
**Group:** ADEP  
**Mentor:** Patrick Nakagawa  
**Category:** Non-Technical  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25832

## **Risk Management in the LANL TRU Program**

In the hopes of helping students and employees understand the process and importance of risk assessment, my poster is going to focus on the risk portion of project management, specifically the process of identifying, assessing the consequences, assessing the magnitude of the consequences, and identifying response actions for a risk. The basic format is going to have the title LTP risk management. The body of the poster will be set up similar to a flow diagram with a description of EP and their Program Management team. After that, will be the description of the 3706 TRU waste campaign. This will help set up the way we are able to identify programmatic risks verses specific risks such as W2, W3, and W4 risks. With that, there will be a box identifying the definition of a risk and also what happens when a risk is identified. Also, with that, there will be a box showing how we are able to quantify and qualitatively examine the risk. The final box will be examples of risks from the programmatic to W4 in the 3706 program.

**Name:** Andrew Gordon  
**Program:** GRA  
**School:** University of Texas- Austin  
**Group:** SRO  
**Mentor:** Matthew Hopkins  
**Category:** Non-Technical  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25648

## **The Plutonium Handbook: Making it Easier for Authors and Researchers**

The focus of this project is to host a digitized version of the 1980 reprint of "The Plutonium Handbook" on the LANL library site and to provide authors and researchers at LANL, and possibly elsewhere, with faster, more accurate access to resources within the handbook via electronic links on the web pages. One of the primary goals of this is to facilitate the development of the 2016 edition of the handbook, which is a significant part of LANL's Plutonium Strategy. It has proved exceptionally challenging to locate many of the references within the book, which further justifies the importance of making such sources available to the user, who may otherwise be unable to locate them. Difficulties encountered during the process may help educate authors and librarians on changes in citation standards in the last 40+ years and how to improve them. Access, usability and aesthetics must also be considered in the website development process.

**Name:** Elandra Roybal  
**Program:** GRA  
**School:** New Mexico Highlands University  
**Group:** W-16  
**Mentor:** Dale Talbott  
**Category:** Non-Technical  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25758

## **Analysis of Insider Threat**

The purpose of this project is to conduct research on insider threat and analysis as it applies to nuclear material security. The research considers insiders broadly to learn from the discipline at large, not limited to the nuclear weapon enterprise (NWE). As such I am conducting a literature review of previous research, case studies, and historical events where a trusted insider chose to engage in violent and criminal activity. The overall goal is to evaluate the psychology of these specific cases, apply psychological theories, and speculate possible explanations of motivation. We will identify potential actions that can be taken to prevent future events, consider motivation, and attempt to identify patterns. As stated in a DOE/NNSA fact sheet released on March 23, 2012, "almost all known cases of theft of nuclear material involved an insider." Therefore researchers are led to believe, "the threat of a nuclear facility insider, either individually or in collusion with an outsider, stealing fissile material or committing sabotage at a nuclear facility is important to consider." The results of this research will support both current and future DOE/NNSA studies that must consider the insider threat to understand overall risk.

**Name:** Adrian Coronado  
**Program:** UGS  
**School:** University of New Mexico

**Name:** M. Gabriella Garcia  
**Program:** UGS  
**School:** University of New Mexico

**Name:** Jesse Giron  
**Program:** UGS  
**School:** University of New Mexico

**Name:** Mariah Urbina  
**Program:** UGS  
**School:** New Mexico State University

**Group(s):** ADEP, BPS-SLS, BPS-AS  
**Mentor:** Patrick Nakagawa, Marlene Martin  
**Category:** Non-Technical  
**Type:** Group Poster Presentation  
**LA-UR:** 13-25833

### **3706 TRU Waste Campaign**

This is to help the students outside of the ADEP directorate to understand what Environmental Programs does, specifically with handling the 3706 TRU Waste Campaign.

**Name:** Emily Schulze  
**Program:** GRA  
**School:** University of Utah

**Name:** Manny Vargas  
**Program:** UGS  
**School:** Northern New Mexico College

**Name:** Gabriel Vigil  
**Program:** UGS  
**School:** Northern New Mexico College

**Name:** Shelby Walker  
**Program:** UGS  
**School:** Trinidad State Junior College

**Group(s):** CAP-FS  
**Mentor:** Mike Alexander  
**Category:** Non-Technical  
**Type:** Group Poster Presentation  
**LA-UR:** 13-25771

## **One Gallon at a Time: A Turning Point for Groundwater Remediation at LANL**

The Associate Directorate for Environmental Programs (ADEP) has been investigating the pathways through which chromium contaminated effluent water has percolated from a wetland ecosystem to the regional aquifer beneath a neighboring canyon in Los Alamos, New Mexico. Initial investigations have paved the way for a “Pump and Treat” ion-exchange process to be performed at existing monitoring wells in Mortandad Canyon, where a large plume of chromium has been detected. In addition, the wetland from which the legacy industrial chromium water originates will be stabilized by a grade control structure to further contain the remaining chromium contaminated soils. These projects represent a turning point for the ADEP Groundwater Program from investigation and monitoring, to remediation and action. Clean water is one of the nation’s most important resources and the work being performed by the Laboratory and its contractors will preserve and protect this valuable source for future sustainable use.

**Name:** Michael Collins  
**Program:** GRA  
**School:** Northeastern University  
**Group:** P-21  
**Mentor:** Michelle Espy  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25763

## **Modeling Coil Configurations for Nuclear Quadrupole Resonance**

Surgically implanted or ingested contraband (e.g. explosives or drugs) is challenging to detect. Nuclear quadrupole resonance (NQR) may be capable of discovering such threats. In NQR, radio frequency magnetic fields (0.5-6 MHz) are applied to a sample in order to determine whether an explosive or other material of interest (MOI) is present within that sample. The radio signal returned by the MOI is typically very weak, therefore it is important that the coil used to excite the sample maximizes this return signal within the design constraints of maximum acceptable power and pulse length. An ideal transmit coil is capable of producing a magnetic field of homogeneous magnitude in the region being examined. Additionally the field magnitude must be sufficiently high that only a short pulse length is required for full sample excitation. A good detection coil must be as sensitive to the return signal as is possible without being overwhelmed by the effects of ringing, electromagnetic interference, or thermal noise. A computer simulation has been developed in MATLAB to help solve this coil optimization problem. It allows the designer to evaluate the detection efficacy of different coil designs and configurations. It predicts, in absolute terms, the level of signal that is expected from an arbitrarily shaped and positioned MOI for a given pulse length and power level. Both single coil (transceiver) designs and separate excitation/detection coil configurations can be tested. The simulation is currently being used to help design a transceiver coil for the single-sided detection of explosive surrogates placed 2-10cm away from the coil. In the future, the simulation may be expanded to include the effects of polarization enhancement.

**Name:** Dana Duke  
**Program:** GRA  
**School:** Colorado School of Mine  
**Group:** LANSCE-NS  
**Mentor:** Fredrik Tovesson  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25803

## **Total Kinetic Energy Measurements of 235-U and 239-Pu (n,f)** **Fission Products**

Most of the energy released in neutron-induced fission goes into the kinetic energy of the resulting fission fragments. Fission theorists have indicated a need for additional average Total Kinetic Energy (TKE) information at incident neutron energies relevant to defense- and energy-related applications, as current measurements are lacking [1]. These data would improve our understanding of the fission process and provide a valuable observable against which simulations can be benchmarked. An experiment will run at the Los Alamos Neutron Science Center (LANSCE), during the 2013 run cycle to measure TKE of fission products following the neutron induced fission of 235-U and 239-Pu over incident neutron energies from thermal to hundreds of MeV. Two independent measurements will be made, one using a double Frisch-gridded ionization chamber, and another employing silicon surface barrier detectors. The experiment setup and exploratory analysis of ionization chamber data will be presented.

### Reference:

(1) D.G. Madland, Total prompt energy release in the neutron-induced fission of 235-U, 238-U, and 239-Pu, Nuclear Physics A 772 (2006), no. 113-137.

**Name:** Sarah Ferguson  
**Program:** UGS  
**School:** Angelo State University  
**Group:** C-PCS  
**Mentor:** Michael Di Rosa  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25214

## **Design of a Magnetic Trap and Accumulator for Laser-Cooled Atoms and Molecules**

Ultracold atomic physics has led to new discoveries such as Bose-Einstein condensates, super fluidity, and super conductivity. Similarly, it is theorized that molecules cooled to ultracold temperatures will lead to new discoveries. Laser cooling is one method that has been shown to cool atoms to ultracold temperatures and can be used to cool molecules as well. Magnetic traps can be used to store ultracold paramagnetic atoms and molecules. Our design for a magnetic trap confines paramagnetic atoms and molecules in a weak-field seeking state between two magnetic potentials generated by a linear configuration of sextupoles and solenoids. Keeping Liouville's theorem in mind, we will optically pump the particles so that they are injected in the strong-field seeking state, and then optically pump them back into the weak-field seeking state for storage once they are in the linear trap. The successful trapping of particles depends on many parameters and conditions such as initial axial velocity and position, initial radial velocity and position, where the state changes occur, the length of the trap, the configuration of the magnets, and strength of the magnetic field. The goal of this research is to determine the possible parameters and conditions that will allow for paramagnetic particles to be injected and accumulated in this linear trap.

**Name:** Timothy Green  
**Program:** UGS  
**School:** Harvard University  
**Group:** XCP-8  
**Mentor:** Robert Chrien  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25497

## **Fractional Energy Losses in ICF Reactions Due to Pusher Collisions**

In inertial confinement fusion (ICF) reactions, a capsule filled with deuterium and tritium fuel is compressed until the deuterium and tritium atoms are ionized and begin to fuse together, creating ions and other products. These product ions are then slowed down due to collisions with the constituents of the fuel, resulting in an increase in the fuel temperature. The energy yield of ICF reactions depends on how much of this self-heating occurs as a result of the slowing down of these product ions. For some of these reactions, these product ions will collide with the capsule wall before depositing all of their available energy, thus reducing the total yield. Though we do currently have a useful model for simulating these reactions, this model ignores these losses completely. By considering where in the capsule these fusion reactions take place, one can place a scaling factor on each reaction's energy deposition to account for these losses. Averaging this expression over all possible directions, one can then arrive at an expression for the expected value of energy deposition for each reaction in terms of distance from the capsule wall.

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**Program:** UGS  
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**Group:** P-25  
**Mentor:** Dale Tupa  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25533

## **Testing a PDV Microphone**

Photon Doppler Velocimetry, or PDV, is a method used for determining the velocity of a moving object with reflected, Doppler shifted laser light. Its high level of sensitivity makes PDV very useful to measure the incredibly high velocities involved in dynamic experiments. This sensitivity may allow PDV to detect subtle undertone frequencies in vibrating objects as a tool for structural analysis and sound recording. To better understand the range of possible applications for and the concepts behind this new technology, multiple designs of a PDV microphone were developed and tested.

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**LA-UR:** 13-25753

## **Radio Frequency Signal Acquisition and Processing**

### Task 1:

The Los Alamos National Laboratory operates an EMP Simulator that provides key support to an important Air Force Mission. Ground data generated by this source have been recorded for the past 12 years. The archive representing this dataset is very large. Although analysis is routinely conducted on these data, the process was neither streamlined nor efficient. New codes were developed to analyze these data and a user-friendly GUI was created in MATLAB. This resulted in a process that allows the dataset to be systematically and efficiently organized and collated.

As part of this task, I gained knowledge of various signal analysis techniques through time domain and basic frequency domain representations of the waveforms. Additionally, I learned how to apply basic digital filtering techniques to a given signal using the MATLAB Signal Processing Toolbox.

### Task 2:

As a secondary task, I acquired hands-on experience in programming and controlling scientific laboratory instruments such as time interval counters, digital delay generators and timing equipment using the MATLAB Instrument Control Toolbox. I also learned to operate handheld oscilloscopes, frequency spectrum analyzers and various antennae. These instruments play a key role in acquiring RF data from various sources.

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**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25579

## **Particle Acceleration and Magnetic Field Amplification in Supernova Remnant Shocks**

The acceleration of cosmic rays is one of the major unsolved problems in astrophysics. Supernova Remnants (SNRs) are widely expected to be the sites for accelerating galactic cosmic rays through the so-called diffusive shock acceleration (DSA) mechanism. Recent observations have indicated that magnetic field is strongly amplified beyond the simple shock compression. The strong magnetic field may have strong implications to particle acceleration and synchrotron X-ray emissions in SNRs. By coupling a state-of-art MHD simulation with a particle transport model, we investigate particle acceleration and magnetic field amplification in a shock-turbulence system similar to a SNR shock propagating into a turbulent interstellar medium. We numerically solve the Parker's transport equation using a stochastic method in which the magnetic and velocity fields come from MHD simulations. We show magnetic field get amplified up to several hundred micro Gauss in the downstream region. Meanwhile, the shocked region is featured by multiple secondary shocks and large-scale velocity variations. Our preliminary results from the particle transport model show that particles get accelerated at the forwarding shock and further accelerated in the downstream region. This result may help understand the production of cosmic rays and X-ray observations for SNRs.

**Name:** Kyle Miller  
**Program:** UGS  
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**Mentor:** Dale Tupa  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25532

## **Analyzing Data from a PDV Microphone**

Photon Doppler Velocimetry (PDV) is used to measure very fast velocities on rapid time scales. We use this technology to measure miniscule vibrations of Mylar in response to a sound wave. We analyze this data to transform from the reflected light signal to velocity of the Mylar sheet. Several steps are used to accomplish this, including Fourier analysis. Finally, the velocity data is converted into a sound file and played back, attempting to replicate the initial sound.

**Name:** John Neal  
**Program:** UGS  
**School:** Pacific University  
**Group:** P-21  
**Mentor:** Pulak Nath  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25507

## **Utilization of Two Phase Interfaces to Recover Magnetic Materials in High Gradient**

High-Gradient Magnetic Separation (HGMS) is the use of a large magnetic gradient to separate magnetic materials from solution. The separation of magnetized particles is valuable within the biopharmaceutical industry, the mineral industry, and for the biofuel industry (algae harvesting). Current protocols is impeded by particle recovery which is not a continuous process for HGMS; it is time consuming and cumbersome. In this work, we consider the introduction of a two phase flow to aid magnetic particle recovery. First an air-liquid interface was used for the recovery of the particles. Using the air-liquid interface magnetic algae was separated and recovered; however, the process is only semi-continuous because the two steps (separation and collection) are done independently. Separation is thus interrupted while the air interface is introduced to remove the magnetic particles. Therefore, we consider a second approach which introduces a liquid-liquid interface of two immiscible fluids. Continuous separation of magnetic particles is presented based on the second approach. This approach allows both steps to run at the same time and avoids the need to interrupt separation to recover the particles.

**Name:** Kimberly Nguyen  
**Program:** UGS  
**School:** University of New Mexico  
**Group:** MPA-CINT  
**Mentor:** Richard Sandberg  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25421

## **Lensless Microscopic Imaging Using a Tabletop He-Ne Laser**

Microscopy is an essential tool for studying the structural composition of various materials and biological specimens. As such, it lies at the foundation of progress for a myriad of scientific fields. The primary goal with regard to microscopy is to develop the ideal microscope, one which holds the ability to produce high-resolution images from nanometer-scale samples at high speeds. Pulsed x-ray sources present a promising method through which the ideal microscope can be created; however, high resolution lenses for these sources are difficult to make and are inefficient. An alternative to lens based microscopy is a technique called lensless imaging or coherent diffraction imaging. The resolution of images produced from this technique is limited only by the illuminating flux on the sample and the wavelength of the illuminating source. In the lensless imaging approach, a highly coherent source such as an optical laser or x-ray free electron laser is focused onto a sample, resulting in diffraction patterns that can be captured by a charge-coupled device (CCD) camera and reconstructed as a high resolution image. The diffraction patterns from the waves are analyzed and transformed into an incoherent image by implementing mathematical computer algorithms that use Fourier Transforms. Through repeated iterations of the technique, paired with isolation of the sample, the amplitude and phase information of the waves can be obtained, allowing for the high resolution image to be reconstructed. We demonstrate a tabletop, helium-neon laser based lensless microscope suitable for undergraduate teaching laboratories.

**Name:** Elise Pusateri  
**Program:** GRA  
**School:** Rensselaer Polytechnic Institute  
**Group:** XCP-6  
**Mentor:** Heidi Tierney  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25455

## **Development of an Electron Swarm Model**

This electron swarm model calculates the evolution of a swarm of electrons that is created by photoelectron ionization of air and Townsend impact ionization at a given air density and electric field. The code uses an adaptive time step and solves a system of coupled differential equations for electric field, electron temperature, swarm electron number density, and drift velocity. In this context, a swarm means that the electrons are in thermodynamic equilibrium with themselves, but not necessarily with the background. We are interested in the amount of time it takes for the newly generated electrons equilibrate to the ambient electric field and pressure to reach a characteristic electron temperature that defines a swarm.

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**Program:** GRA  
**School:** Brigham Young University  
**Group:** EES-17  
**Mentor:** Brian Anderson  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25699

## **Imaging Stress Corrosion Cracking in Steel Using Time Reversal Techniques**

Stress corrosion cracking (SCC) is an important failure mechanism that is of concern for long term storage of canisters containing spent nuclear fuel. In this application SCC may be developing over many years and a nondestructive method to locate and prognosticate failure at locations on the canister is required to ensure safe storage of spent fuel. In seeking a way to nondestructively test the strength at specific locations, it is essential that known representative cracks be carefully studied. By using a technique called time reversal, one can focus localized energy at specific points in space on a surface and at a specific orientation to inspect a piece of metal point by point. After creating focused waves of different amplitudes at the same location, comparisons of the focal signals can be made at the different amplitudes to quantify potential nonlinearities. These nonlinearities point to the presence of cracks in the material since cracks have been shown to vibrate in a nonlinear fashion at sufficient amplitudes (note that these amplitudes are still considered small enough for the testing to remain nondestructive in nature). It is hoped that by conducting this technique at various frequencies, more information can be gathered about the size, depth, and orientation of the crack. A stainless steel plate with known cracks due to SCC was inspected in order to discover the viability of using various frequencies in imaging a crack's size and depth information. The results from various time reversal experiments used to locate nonlinearities and therefore cracks will be presented. [This work was supported by the U.S. Dept. Of Energy, Fuel Cycle R&D, Used Fuel Disposition (Storage) Campaign.]

**Name:** Christopher Romick  
**Program:** GRA  
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**Group:** WX-9  
**Mentor:** Tariq Aslam  
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**Type:** Individual Poster Presentation  
**LA-UR:** 13-25415

## **Inherent Length Scales in Gaseous Hydrogen-Air Detonation**

The development and propagation of gaseous Hydrogen-air detonations are examined using a temporally and spatially resolved power deposition to initiate a reaction wave. For this examination, both the reactive Euler and Navier-Stokes equations with Arrhenius kinetics are solved in one dimension. The behavior of a simplified model using one-step kinetics as well as a detailed hydrogen-air mechanism is examined. The use of a detailed hydrogen-air mechanism gives rise to intrinsic lengths that span many orders of magnitude in a steady detonation. For an accurate prediction of the behavior, the finest scale present must be resolved while still capturing the engineering scale. To simplify this difficulty, the simpler one-step model was examined as it has only one steady length scale. Even within the simple one-step kinetics model, the propagation of the detonation can present a wide range of scales. Though the results of the inviscid detonation are qualitatively similar to the viscous detonation, there are quantitative shifts in the behavior. The effect of diffusion is more definitive when larger diffusive coefficients are used. Resolving the range of scales present in either the detailed kinetics or the simple one-step model using a uniform grid is very computational expensive, even in one dimension. However, the cost can be reduced in two ways. First, utilizing an operator split between advection, as well as diffusion and reaction allows for large overall time-steps to be taken with sub-steps taken only for diffusion and reaction. Moreover, using the Wavelet Adaptive Multi-resolution Representation (WAMR), the number of points necessary to accurately represent a flow field can be dramatically reduced. This methodology has recently been expanded to parallel computing environments thus enabling a quicker physical time to the same simulation time.

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**Program:** UGS  
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**Group:** WX-9  
**Mentor:** Dana Dattelbaum  
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**Type:** Individual Poster Presentation  
**LA-UR:** 13-24674

## **The Shock Sensitivities of Nitromethane/Methanol Mixtures**

Understanding the detonability limits of explosives is of critical importance for the safe handling and transportation of explosives and related chemical commodities. It is also of interest for the fundamental detonation physics of how diluents influence shock sensitivity and resultant reactive flow, including detonation velocities, pressures, reaction zone lengths, and detonation wave stabilities. Quantifying detonability is challenging because the critical diameter rapidly increases with % diluent.

**Name:** Erik Shaw  
**Program:** UGS  
**School:** Middlebury College  
**Group:** P-23  
**Mentor:** Michael Ronquest  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25510

## **SLIMER - Scintillator-Layered Imaging Microscope for Environmental Research**

The goal of SLIMER is to image  $^{14}\text{C}$  in biological samples from permafrost from the McGill Arctic Research Center (MARS) using CsI scintillation material and a microscope attached to an electron-multiplying charge-coupled device (EMCCD). The application of this technique will help determine the ingestion rate of the microbial community of organic carbon and will allow a better understanding the effect melting permafrost will have on the environment in the long run. We have imaged higher energy alpha and gamma sources like  $^{241}\text{Am}$  and  $^{207}\text{Bi}$ , but low energy beta emitters like  $^{14}\text{C}$  and  $^{90}\text{Sn}$  are challenging to image.  $^{14}\text{C}$  has not been detected using this method previously. So far I have developed from scratch software used to analyze the data and become competent in the use of the experimental apparatus. The existing software will now be used to search for lower energy gamma and electron events and refined to detect the low energy  $^{14}\text{C}$  events.

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**Program:** GRA  
**School:** Colorado School of Mines  
**Group:** LANSCE-NS  
**Mentor:** Fredrik Tovesson  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25813

## **The Development of the New SPIDER Detector at LANSCE**

Fission product yields (FPY) are crucial to a better understanding of the fission process. These data impact our modeling of next generation nuclear power and our confidence in the current stockpile. A small and partially conflicting set of FPY experimental results at higher than thermal neutron energies for critical actinides in ENDF and other nuclear libraries produces a need for new precision measurements.

The SPIDER (SPectrometer for Ion DEtermination in fission Research) detector is being developed at LANSCE-WNR (Los Alamos Neutron Science Center - Weapons Neutron Research) to fill this need. The detector will have exceptionally high fragment mass and incident neutron energy resolution allowing for unprecedented measurements of the FPY directly after fission takes place.

An overview of the detector components, data acquisition system, simulations, and preliminary test results will be presented.

**Name:** Corinne Silkwood  
**Program:** UGS  
**School:** New Mexico State University  
**Group:** LANSCE-LC  
**Mentor:** Katharine Page  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25221

## **Decahedral Nanoparticles: Can PDF Measurements Settle the Controversy?**

Dodecahedral metal particles have been observed since their discovery by Ino in 1966. Decahedral particles are believed to be comprised of fivefold twinning (also called “multiple twinning”) of tetrahedral subunits across the  $\{111\}$  planar surfaces of the face-centered cubic (FCC) lattice. The angle between sides of equilateral tetrahedra is about 70.53 degrees; consequently, five-fold twinning around a central axis spans only  $352.65^\circ$ , leaving a  $7.35^\circ$  gap in the structure. The questions raised by this spatial discontinuity, relative to the internal atomic structure of the particle, have been the subject of a half century debate. Difficulties in characterizing the structure of the nano-morphologies are due in part to the weak contrast offered by strained lattices in electron microscopy and the broadening of Bragg peaks due to size effects in diffraction experiments. We examine the feasibility of applying atomic pair distribution function methods utilizing total scattering data to determine the atomic structure of decahedral nanoparticles. We consider three proposed models for twinned decahedral nanoparticles: (1) A model assuming no lattice distortions or deformation, resulting in a solid angle gap of 7.35 degrees. The gap may consist of a solid wedge missing from the particle or may be distributed between subsequent tetrahedral subunits; (2) A model with an orthorhombic lattice, allowing the particle to adopt fivefold symmetry without gaps. The original fcc lattice parameters are deformed such that angle between sides of the tetrahedra increases to  $72^\circ$  while maintaining close packing; and (3) A hybrid model which includes a combination of FCC structure subunits and transformed orthorhombic subunits. We calculated the diffraction and pair distribution function data corresponding to each model and compared them with simulated data from spherical FCC particles. Our results present the feasibility of using atomic PDF measurements to assess the accuracy of the proposed models for multiply twinned nanoparticles.

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**Program:** UGS  
**School:** Northern New Mexico College  
**Group:** P-25  
**Mentor:** Dale Tupa  
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**Type:** Individual Poster Presentation  
**LA-UR:** 13-25632

## **A Prototype PDV System for Use at the Proton Radiography Facility**

PDV (Photon Doppler Velocimetry) is a diagnostic to measure the velocity of a moving surface. A laser illuminates the object and we gather light reflected off of the surface of that object. The reflected light has a different frequency than the impinging light because of the Doppler shift caused by the moving surface. We gather the shifted and the un-shifted light to determine the beat frequency and use it to measure the velocity of the surface. As part of the Velocimetry team at Proton Radiography (pRad), we built a prototype PDV system from scratch and tested it, along side of a proven PDV system that has been used in previous experiments at pRad. Our new system will be used as a model for future less expensive PDV units for the pRad facility.

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**Program:** GRA  
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**Group:** ISR-2  
**Mentor:** Kalpak Dighe  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25748

## **Radio Frequency Signal Detection and Analysis**

Task 1: Radio frequency (RF) energy radiates from a conducting surface into free space, and travels long distances as an electromagnetic wave. As a practical application, almost every wireless technology from cell phones, TV and radio broadcast utilizes radio frequencies to communicate information via radio waves. However, many impulsive electrical discharge processes such as lightning or on/off switching of high current devices, emit broadband RF energy as a secondary product. In the time domain, a fast rise time event will result in a large frequency bandwidth emission, while a slow rise time will result in a narrower bandwidth emission. The focus of this research is to process, analyze and characterize signals detected from one such extremely fast rise time event (hence large bandwidth).

The event took place in an RF rich environment; thus, it was vitally important to identify unique signals emitted by the source as opposed to those from the prevalent background. This task was performed both in the time as well as frequency domain by applying the fast Fourier transform analysis. Spectrograms were generated and key attributes of the signals (polarization, bandwidth, temporal persistence, etc.) were examined to obtain valid results that will be presented in this poster.

Task 2: As a secondary task, I acquired hands-on experience in programming and controlling scientific laboratory instruments such as time interval counters, digital delay generators and timing equipment using the MATLAB Instrument Control Toolbox. I also learned to operate handheld oscilloscopes, frequency spectrum analyzers and various antennae. These instruments play a key role in acquiring RF data from various sources.

**Name:** Lorenzo Venneri  
**Program:** UGS  
**School:** Rice University  
**Group:** XCP-6  
**Mentor:** Tierney Heidi  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25472

## **Non-Equilibrium Air Chemistry For Lightning Using Exponential Euler Methods**

Lightning is a complex multi-physics and multi-scale phenomenon. Progress has been made understanding some aspects of its initiation, development, and stages with necessarily limited physical models. This work focuses on improving the air chemistry treatment that is used in lightning and laboratory discharge models at LANL. In particular, we examine the dominant reactions that take place in an atmosphere that is characterized by electric field and pressure. We choose pertinent species and reactions to create a reaction model that follows the concentrations of air species with ongoing time. Each reaction has an associated differential equation based on the probability of the reaction occurring. We test several numerical methods to solve these differential equations given normal initial conditions for air (STP, 78% N<sub>2</sub>, etc) and find forms of the exponential Euler method to be most accurate. The results are interesting on the nanosecond scale and can be compared with experimental data. We find, in a simplified run, that diatomic Nitrogen and Oxygen dominate the air chemistry although other species grow in concentration and stabilize. Also, when compared to other experimental electron production rates, our model shows similar trends. This work will be used as a module to fluid discharge models that currently only track bulk charged species motion. In addition, it will help us better understand the importance of non-equilibrium air ionization processes in other LANL codes.

**Name:** Bryan Zeck  
**Program:** GRA  
**School:** North Carolina State University  
**Group:** P-25  
**Mentor:** Mark Makela  
**Category:** Physics  
**Type:** Individual Poster Presentation  
**LA-UR:** 13-25692

## **A System to Study Electron Trajectories in Ultracold Neutrons A (UCNA)**

The UCNA experiment measures the free polarized neutron beta-decay neutron spin-electron momentum asymmetry parameter,  $A$ , by holding ultracold neutrons in a material trap in a strong magnetic field. The charged particles emitted in a beta-decay then travel along the magnetic field lines until they reach detectors, which provide position and energy information. In these experiments, it is necessary to precisely measure the time of flight of particles relative to their energy and initial angle in order to understand the effects of magnetic field non-uniformity. The use of an avalanche photo-diode detector (APD) with a Sn-113 source attached to it functions as a tagged source, with the 360 keV conversion electron emitted coincidentally to a 20 keV Auger electron. The Auger electron, captured by the APD, allows the time of flight to the detector of the 360 keV electron to be measured to nanosecond precision. This measurement will resolve uncertainties in the UCNA experiment simulation. This represents one of the final essential components of a strategy to produce a 0.2% total uncertainty measurement of asymmetry parameter  $A$ .

**Name:** Erik Edelmann  
**Program:** UGS  
**School:** Cornell University

**Name:** Zoe Martin  
**Program:** UGS  
**School:** University of New Mexico

**Group(s):** XTD-2  
**Mentor:** Leslie Sherrill  
**Category:** Physics  
**Type:** Group Poster Presentation  
**LA-UR:** 13-25461

## **Reshock Mix Experiments: Data Analysis and Comparison to RAGE Simulations**

A recent experiment to study the physics of reshocked materials was performed at the OMEGA laser facility. The goal of this experiment was to help provide detailed quantitative data to help validate and improve the BHR-2 mix model in the RAGE hydrodynamics code. In this poster, we will present both the analysis of titanium experimental data and the corresponding simulations. Similar post-processing tools were used to compare the mix widths of the simulations and the experimental data for a range of times. In addition, a method of extracting a mix area was developed for both the simulations and the experimental data. With the mix area studies, several factors were analyzed, including the prominence of streaming features behind the mix layer. Several parameter studies were also conducted using the simulations, including varying coefficients in the BHR-2 mix model and ultimately comparing to the experimental data.

**Name:** Ashlynn Daughton  
**Program:** GRA  
**School:** University of California- Berkeley  
**Group:** B-11  
**Mentor:** Armand Dichosa  
**Category:** Biosciences  
**Type:** Technical Talk  
**LA-UR:** 13-25694

## **The Ninety-Nine Percent of Unculturable Bacteria**

Fewer than 1% of bacteria are readily cultivated using traditional laboratory techniques. This is problematic for microbiologists and environmental biologists attempting to understand the diversity and dynamics of complex bacterial communities. Several culture-independent tactics have been developed in the recent past to circumvent this problem. One tactic is to use culture-independent metagenomics to classify the representatives of an environmental microbial community and infer a functional profile. Unfortunately, metagenomics does not typically uncover the rare species that may still play an important ecological role. Another culture-independent approach is single cell genomics, where a single bacterial cell is isolated and sequenced. However, due to insufficient DNA template, typically < 60% of the genome can be determined. To simultaneously chase after rare community members and improve genome recovery above that of a single cell, our group is investigating gel microdroplet technology. We encapsulate single cells in agarose-based gel microdroplets (GMDs) and incubate them in-situ or in media. Because they are physically separated but grown with its native community members, the single cells can grow into clonal microcolonies within the GMD. The GMDs are isolated by flow cytometry and the DNA contained inside is amplified. Because there is more than one clonal cell, amplified DNA can produce high quality, and nearly complete, genomes of novel bacterial species. This talk will present an overview of various GMD applications in environments like the human oral and gut microbiomes, freshwater, and soil communities.

**Name:** Tarryn Miller  
**Program:** UGS  
**School:** Colorado School of Mines  
**Group:** MPA-MSID  
**Mentor:** David Fox  
**Category:** Biosciences  
**Type:** Technical Talk  
**LA-UR:** 13-24803

## **Ionic Liquids as Tunable Solvents for Biofilm-Forming Pathogen Neutralization**

Ionic liquids (ILs) and deep eutectics (DES) are molten salts that are increasingly recognized as suitable materials for multiple biological applications. This is due to their unique physicochemical properties, which can be fine tuned through varying the anionic and cationic components. By simply altering the hydrophobic and hydrophilic properties, viscosity, and conductivity, the new IL/DES can result in novel biological applications. Our team has formulated (synthesized) and tested a panel of ILs and DES for their ability to disrupt the extracellular matrices of these biofilm-forming microorganisms and test their potential as transdermal drug delivery agents. Biofilm-protected microorganisms are thought to be responsible for up to 65% of all bacterial infections in humans and are typically 50-500 times more resistant to antimicrobials than unprotected (planktonic) bacteria, demonstrating their clinical relevance. We hypothesize that the IL or DES formulations will dissolve the extracellular matrix exposing the bacterial cells to an antimicrobial agent. Our studies began with the proof-of-concept pathogens, *Pseudomonas aeruginosa* and *Salmonella enterica* serovar typhimurium LT2, in order to ascertain efficacy of IL-based biofilm-disruption and corresponding cell death. Both 24 and 72 hour biofilms, for each species, were challenged for two hours with each IL or DES in our panel and their corresponding controls and cell viability assessed by enumeration. Concomitant to this work, the same ILs were also tested for irritation, permeation (transdermal delivery), drug release kinetics (from IL to media), and cytotoxicity properties against normal human epithelial cells and skin cells.

**Name:** Joseph Torres  
**Program:** GRA  
**School:** University of Oregon  
**Group:** MST-7  
**Mentor:** Michael Blair  
**Category:** Chemistry  
**Type:** Technical Talk  
**LA-UR:** 13-25597

## **Optical Analysis of Ce<sup>3+</sup> Doped Borate Glass**

Glasses are defined as super cooled liquids, and possess transparency with amorphous structure. SiO<sub>2</sub> and B<sub>2</sub>O<sub>3</sub> are commonly used as glass formers for commercial glass preparation. Borate glasses are an attractive host because of their low viscosity, low melting temperature, and high stability. Borate glasses doped with Ce<sup>3+</sup> are synthesized and their structural, thermal, optical absorption, and photo luminescence properties were measured using X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), FT-IT, Differential Scanning Calorimetry, and optical absorption techniques. XRD and SEM was utilized to confirm the amorphous nature of the glass. FTIR was performed to identify the functional groups of the glass matrix. DSC was utilized to determine the glass transition (T<sub>g</sub>). Using different heating rates, the activation energy of the glass was determined. The Ce<sup>3+</sup> doped glasses show spectrally broad 5d → 4f luminescence in the violet-blue (centered around 360nm) under both direct optical excitation of Ce<sup>3+</sup> at 321 nm. The decay lifetime of the Ce<sup>3+</sup> doped glasses was also measured.

**Name:** Mitchell Wood  
**Program:** GRA  
**School:** Purdue University  
**Group:** T-1  
**Mentor:** Marc Cawkwell  
**Category:** Chemistry  
**Type:** Technical Talk  
**LA-UR:** 13-24754

## **Spectroscopic Characterization of Explosive-Binder Interfaces via Quantum MD**

High explosives are a plastic-bonded composite of an energetic molecular crystal in a polymer matrix. The interface between the energetic molecular crystal and polymer binder controls the adhesion of the composite, among other properties. We have used quantum-based molecular dynamics (QMD) simulations to characterize the vibrational spectra of the interface between the explosive RDX and polyethylene as a function of the surface plane of the RDX single crystal. QMD provides a very accurate, self-consistent, and transferable description of interatomic bonding in organic materials but its considerable computational expense has limited applications to only small systems. QMD on hundreds to thousands of atoms is not tractable owing to recent algorithmic developments in the LANL-developed code LATTE. These advances include the removal of the expensive self-consistent field optimization and the computation of the density matrix in parallel on multiple graphics processing units. Thus, in a computational first, we have been able to extend QMD simulations out to hundreds of picoseconds for a thousand atoms, both of which are needed for collection of vibrational spectra on these composites. With these new capabilities we have predicted shifts in vibrational spectra that depend on the crystallographic orientation of the interface RDX and polyethylene that will guide subsequent experimental studies.

**Name:** Christopher Armstrong  
**Program:** UGS  
**School:** New Mexico Tech  
**Group:** XTD-1  
**Mentor:** Wayne Weseloh  
**Category:** Computing  
**Type:** Technical Talk  
**LA-UR:** 13-25810

## **Shaped Charge Analysis Using Pagosa**

Shaped charges have been in use since WWII in many different applications like armor-penetrating weapons, cutting metal, demolition, and well perforation. A shaped charge is a mass of explosives with a specifically shaped cavity lined with metals or alloys based on the desired effect and target. There was a lot of research done in the 1950's regarding shape charges and how they function. Today's analysis of shape charges and other high explosives applications can be done using hydrocodes. Hydrocodes are used to model the fluid like behavior of rigid materials when plastically deformed due to high strain rates. This project compared some properties of shaped charges found experimentally in the 1950's to computer models produced today. These properties include liner velocity, slug velocity, jet velocity, mass of the slug, mass of the jet, and surface temperature. Other properties that computer modeling allows us to analyze that cannot be done experimentally are properties such as pressure and internal temperature. The shaped charge used in this problem was bare conical shaped charge with a copper liner. The hydrocode used to model this was Pagosa. Pagosa uses a large amount of Eulerian type calculations to model the flow of materials throughout the mesh.

**Name:** Anthony Pearson  
**Program:** UGS  
**School:** St. Cloud State University  
**Group:** HPC-1  
**Mentor:** Jorge Roman  
**Category:** Computing  
**Type:** Technical Talk  
**LA-UR:** 13-25406

## **Introducing Artificial Neural Networks to Entity Disambiguation**

The human brain, according to most research, contains around 100 billion neurons. While human understanding of the world and the objects in it are complex, creating a model to conceive the way we distinguish those objects is vastly complex. The research in “Entity Disambiguation Using Semantic Networks” used a framework and hand constructed weights for disambiguating authors that is based on connectedness using triples, or subject-predicate-object expressions<sup>1</sup>. Connections are representations of knowledge extracted from bibliographic records that may contain names, affiliations, dates, and themes. The count and type of connections between the entities in question are necessary to see if they are strongly connected, which implies that they are the same. This article explains how to introduce artificial neural networks for general entity disambiguation. In this case, semantic networks are used to gather input for the artificial neural network. The artificial neural network learns from previous examples using weights and uses the weights to generalize unseen sets of weights to give a educated answer. If it is true, that an entity is co-referent, else false, it is not. Furthermore, the article concludes with observations and future work. The work that has been already done can be extended to disambiguate different entities, such as organization. The overall goal of the research is to find a pattern between types entities and come up with a general process, instead of writing heuristics that finds connections between entities. The use of entity disambiguation with artificial neural networks are necessary to a greater intelligence in machine learning.

**Name:** Phillip Shaw  
**Program:** UGS  
**School:** University of New Mexico  
**Group:** NIE-CS  
**Mentor:** Carl Knauss  
**Category:** Computing  
**Type:** Technical Talk  
**LA-UR:** 13-25689

## **NIE Network Operation Center's Cacti Project**

Laboratory mission objectives require a reliable and robust network environment, which also includes telephony, which affects both classified and unclassified resources: physical security, environmental sensors, and providing the infrastructure for building automation functions. In supporting the lab's mission with the current Nortel/Avaya switching infrastructure has meant hurdling new obstacles as both technology and expectations change. The Network Operations Center's (NOC) Cacti project is an effort to improve network reliability and shorten troubleshooting time by collecting and archiving data from predefined metrics, which is useful in establishing baselines and trends across a given timeline and help troubleshoot bandwidth limitation, network loops, multicast flooding, etc. These goals are accomplished today by an open source application called Cacti, developed and deployed to the production network environment this year. With this application, network devices are added to the Cacti database, monitored and polled, collecting statistics from each device and then plotted on a customized graph providing an illustration for both engineers and users. Illustrations may be used as a means of reporting for Departmental Computing Support (DCS) technicians for a particular issue, or for other entities that may require validating a Service Level Agreement (SLA).

**Name:** Zachary Butterfield  
**Program:** UGS  
**School:** Utah State University  
**Group:** EES-14  
**Mentor:** Manvendra Dubey, Rodic Lindenmaier  
**Category:** Earth and Space Science  
**Type:** Technical Talk  
**LA-UR:** 13-25640

## **Total Column Observation of Nitrogen Dioxide in the Four Corners Region**

In the Four Corners Region, the San Juan and Four Corners power plants produce 0.2 and 0.1 kilotonnes per day, respectively, of  $\text{NO}_x$  (combined Nitric Oxide (NO) and Nitrogen Dioxide ( $\text{NO}_2$ )) from burning fossil fuels. As  $\text{NO}_2$  is itself a pollutant and drives production of ozone, another tropospheric pollutant, through reactions with hydrocarbons in sunlight, quantifying atmospheric levels of  $\text{NO}_2$  is key to understanding overall regional air quality. We compare  $\text{NO}_2$  column data obtained using a ground-based solar spectrometer (Pandora) and the satellite-based Ozone Monitoring Instrument (OMI) from June 2012 through January 2013. Both instruments compare reasonably well and show similar trends over the six-month period. We plan next to similarly compare ozone measurements obtained using Pandora and a ground-based Brewer Spectrophotometer with ozone measurements from OMI.

**Name:** Amy Jordan  
**Program:** GRA  
**School:** New Mexico Tech  
**Group:** New Mexico Tech  
**Mentor:** Philip Stauffer  
**Category:** Earth and Space Science  
**Type:** Technical Talk  
**LA-UR:** 13-25820

## **Simulation of Radionuclide Gas Breakthrough from Underground Nuclear Explosions**

In the event of a clandestine underground nuclear test, the detection of signature radionuclide gases could help verify the nuclear nature of the explosion. The ability to predict the timing of late-time gas seepage at or near the surface provides an important tool for the international nuclear event monitoring community. Breakthrough of isotopic gas at the surface depends on the device yield, isotope half life, and migration/attenuation factors in the subsurface. In this work, we have developed a two-dimensional, isothermal numerical model for late-time gas migration through fractured porous media in the unsaturated zone following an underground nuclear explosion (UNE). The model is used to perform Monte Carlo simulations to analyze the relative importance of unknown geologic parameters, initial gas distribution, and the effects of structural damage in the subsurface explosion environment (cavity, rubble chimney) on radionuclide breakthrough. Results from the numerical model are compared with experimental data from the NNSS for validation purposes. The model is then used to predict the hypothetical timing and window of opportunity for Xe-133 gas detection from an UNE in rock similar to that of Rainier Mesa and the NNSS, with breakthrough times for Xe-133 ranging from 13 to 51 days following the explosion and the window of opportunity for gas sampling lasting from 37 to 135 days. The results of this study will be used to refine prediction capabilities for the detection of gases from suspected UNEs in other geologic settings.

**Name:** Elizabeth Fischer  
**Program:** UGS  
**School:** University of Texas- Austin  
**Group:** MPA-MSID  
**Mentor:** Kathryn Berchtold  
**Category:** Engineering  
**Type:** Technical Talk  
**LA-UR:** 13-25589

## **Optimizing Tetra-PEG Ion-Gel for Carbon Dioxide Gas Separations**

As the levels of carbon dioxide in the atmosphere continue to rise, new and more efficient methods need to be created to remove carbon dioxide and other greenhouse gases from combustion emission streams. Ionic liquids have high solubility and selectivity for carbon dioxide and would present an appealing option for separations if they could be engineered to efficiently and economically remove carbon dioxide selectively from flue gas. One way this could be done would be to create a polymer membrane to hold the ionic liquid. This membrane must not adversely affect the gas separation properties of the ionic liquid it holds and must also have a high permeability while maintaining high enough strength to be stable during pressure changes that can occur during gas separations. Tetra-arm poly(ethylene glycol) (Tetra-PEG) polymers were synthesized from two different Tetra-PEG monomers with arms of the same molecular weight, containing either amino or succinimidyl reactive end groups. These monomers will be mixed and chemically cross-linked in solution of 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide to create a homogeneous polymer network using different weight percentages of Tetra-PEG and the ionic liquid. Attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy was used to determine information about the distribution of the ionic liquid within the Tetra-PEG membrane. In situ ATR-FTIR spectroscopy of membranes undergoing thermal treatment displayed how the ionic liquid distribution varied with changes in temperature and ionic liquid loading. Gas permeation testing was used to demonstrate how the molecular weight of the Tetra-PEG monomers and weight percentage of the polymer in the membrane affected membrane selectivity and permeability. The results of these tests, to date, and their impact on membranes used for gas separations will be discussed.

**Name:** Ryan Gillis  
**Program:** UGS  
**School:** Brigham Young University  
**Group:** MPA-MSID  
**Mentor:** Technical Talk  
**Category:** Engineering  
**Type:** Technical Talk  
**LA-UR:** 13-25448

## **Optimizing Polymer/Ionic Liquid Composite Membranes for Gas Separations**

Rising levels of carbon dioxide in the atmosphere and growing political momentum make clear the need for new methods to remove greenhouse gases from combustion emission streams. Selectively permeable membranes present an economically appealing choice if they can be engineered to provide sufficient permeability while maintaining high carbon dioxide selectivity. A variety of experiments were performed with the goal of understanding and optimizing membrane characteristics. Membranes were synthesized using a solution casting technique, creating polymer/ionic liquid composites of poly(vinylidene fluoride-co-hexafluoropropylene) and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide with tailored composition. Attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy was used to gain detailed information about the nature of the distribution of ionic liquid and polymer in the membranes. In situ ATR-FTIR scanning of membranes undergoing thermal treatment revealed how the ionic liquid distribution within the membrane was affected by the annealing process. Gas permeation testing demonstrated how co-polymer composition and molecular weight affected membrane permeability and selectivity. The influence that ionic liquid chemistry and content within the composite had on permeability and selectivity was also examined. The results of these tests, to date, will be discussed along with their impact on future membrane technology.

**Name:** Naveen Prakash  
**Program:** GRA  
**School:** Virginia Tech  
**Group:** NEN-5  
**Mentor:** Cetin Unal  
**Category:** Engineering  
**Type:** Technical Talk  
**LA-UR:** 13-25297

## **Peridynamic Simulation of Fracture in Nuclear Fuel Rods**

The linear momentum equation in classical continuum mechanics is a partial differential equation, containing derivatives of the displacement field. It is therefore ill-suited for direct application to problems with discontinuities like fracture problems as the derivatives of the displacement field cannot be defined.

An alternative formulation called Peridynamics was proposed recently which is applicable on or off discontinuities like crack surfaces. This is a Lagrangian nonlocal integral formulation which allows for treatment of fracture in a straightforward manner. In the linear momentum equation, the internal force operator (divergence of stress) is replaced by an integral of forces over a small region surrounding a material point called the horizon. Hence internal forces which are pair-wise in nature, act over finite distances. Each pair-wise interaction is called a bond, and failure is included by allowing bonds to break irreversibly.

In the present research, firstly the effectiveness of peridynamics to predict fracture is investigated. Benchmark problems of fracture are simulated using a code which is under development at Sandia called Peridigm. Simulations are conducted to produce characteristics of dynamic fracture like crack speed, crack branching and crack angle. These are compared against experimental results and simulations using finite element methods. Secondly, Peridigm is used to investigate fracture in nuclear fuel rods. The rod is assumed to be made of a perfectly brittle thermoelastic material. Knowing the evolution of temperature in the rod over time, the displacement field of the rod is calculated using classical continuum mechanics.

**Name:** Mathew Cherukara  
**Program:** GRA  
**School:** Purdue University  
**Group:** INST-OFF  
**Mentor:** Edward Kober  
**Category:** Materials Science  
**Type:** Technical Talk  
**LA-UR:** 13-25095

## **Shock Induced Chemistry of Ni/Al Nano-Composites**

Intermolecular reactive composites find diverse applications in defense, microelectronics and medicine, where strong, localized sources of heat are required. However, there is little knowledge regarding the mechanism of their propagation, which is a roadblock to their widespread application. Recent experimental work has shown that high-energy ball milling can significantly improve the reactivity as well as the ease of ignition of Ni/Al intermetallic composites. Ball milling a mixture of ductile materials like Ni and Al leads to the formation of an intimately mixed nanostructure of Ni/Al that shows increased sensitivity for initiation. Significant reduction in both ignition temperature, which can be as low as 600 K and the threshold impact energy have been observed. However, neither the rationale behind the surprisingly low impact energies for these nano-engineered composites, nor the mechanism of the reaction's propagation is well understood. We present massive (~41 million atom) molecular dynamics simulations of shock-induced chemistry in porous, polycrystalline, lamellar Ni/Al nano-composites, which are designed to capture the observed microstructure post milling. We describe the importance of pores as sites of initiation, where local temperatures can rise to several thousands of degrees, and chemical mixing is accelerated by vortex formation and jetting in the pore. An analysis of the grain deformation in this nano-layered system reveals a multitude of defect mechanisms, viz., Shockley partials, dislocation loops, twinning and the ejection, pinning, elimination and reflection of dislocations at the Ni/Al interface. We also follow the evolution of the chemistry after the shock passage by allowing the sample to 'cook' under the shock induced pressures and temperatures for up to 0.5 ns. Multiple reaction fronts, born in the cauldron of the pores, propagate rapidly through the sample, consuming it within a ns.

**Name:** Stephanie Edwards  
**Program:** GRA  
**School:** University of Oregon  
**Group:** MST-7  
**Mentor:** Dominic Peterson  
**Category:** Materials Science  
**Type:** Technical Talk  
**LA-UR:** 13-25504

## **The Use of Dendrimers in Supercapacitors**

Supercapacitors have a wide variety of uses in everyday life from starters, to hybrid cars, to toys. They possess an extremely high capacitance which makes them suitable for both high and low power activities. While supercapacitors have a very high power density, they unfortunately have a low energy storage density which only allows them to store a fraction of what the average battery can. If the energy storage density were to be increased it would improve the way that mass amounts of energy could be stored and released. Energy density depends on the electrode-electrolyte interfacial area. By engineering an electrolyte solution to cover the entire range of pore sizes present in the electrode, the energy storage density can be increased. This research is focused on adding dendrimers, specifically poly (amido amine) or PAMAM, to the electrolyte solution to give it the dispersity that it needs to contain. The unique structure of dendrimers allows for a wide variety of pore sizes and high charge densities. By adding dendrimers to the electrolyte solution, it may be possible to tailor the electrolyte solution to the electrode. The degradation of the dendrimers was studied using gel permeation chromatography (GPC) along with electrochemical cycling to determine the practicality of using these molecules in supercapacitors. Nuclear magnetic resonance (NMR), x-ray reflectivity (XRR) and neutron reflectivity (NR) will also be used in the future to examine the molecular interactions and determine if dendrimers will solve the energy storage issue.

**Name:** Robin Pacheco  
**Program:** GRA  
**School:** New Mexico Tech  
**Group:** MST-7  
**Mentor:** Dominic Peterson  
**Category:** Materials Science  
**Type:** Technical Talk  
**LA-UR:** 13-25683

## **The Thermal Stability Study of Polybenzimidazole Filled Sylgard 184 Insulators**

The objective of this study was to optimize the thermal performance of polybenzimidazole (PBI) filled Sylgard® 184 (Sylgard) insulators. The current study focused on improving and evaluating thermal properties such as the decomposition temperature using TGA, the glass transition temperature (T<sub>g</sub>) using DSC, and the coefficient of thermal expansion using a dilatometer. PBI/Sylgard composites were first fabricated using range of different particle concentrations (0-1wt %) and curing temperatures (50, 75, 100°C) to determine when the thermal properties were optimized. The optimal particle concentration was estimated by mechanically testing the specimens and determining when the Young's Modulus (E) plateaued. Different curing temperatures were also investigated to ensure that the PBI particulates were uniformly dispersed throughout the matrix. After proper fabrication of the PBI/Sylgard 184 composites, thermal analysis was performed. Results showed the optimal particle concentration was estimated to be 0.5wt% of PBI and the optimal curing temperature was 75°C. The TGA results showed 0.5wt% PBI improves the thermal stability of the composite by allowing it to withstand higher temperatures without decomposing as fast as unfilled Sylgard 184. The DSC results determined the 0.5wt% composite has the greatest T<sub>g</sub> of 326.38°C. Although, the DSC results did not display the plateau trend after 0.5wt% PBI and further DSC testing should be performed to investigate why this trend is not occurring. Future work will consist of determining the thermal conductivity and heat capacity, at temperatures of common use and interest, using Modulated-Temperature DSC (MTDSC). If improvement is successful, PBI/Sylgard composites can be an alternative material for insulation and insulating potting materials at high temperatures.

**Name:** Stephen Parker  
**Program:** GRA  
**School:** University of California- Berkeley  
**Group:** MST-7  
**Mentor:** Andrew Nelson  
**Category:** Materials Science  
**Type:** Technical Talk  
**LA-UR:** 13-25686

## **Oxidation Kinetics of Candidate Cladding Materials under LOCA Conditions**

Zirconium-based cladding alloys have been shown to have favorable neutronic, mechanical and corrosion properties for nuclear fuels operating under normal conditions in a light water reactor (LWR). However, during accident scenarios, such as loss-of-coolant-accidents (LOCAs), the cladding temperature can exceed 1000<sup>0</sup>C; at such elevated temperatures, and in the presence of steam, Zirconium based alloys degrade, lose mechanical integrity, and undergo an exothermic reaction which generates hydrogen. In order to reduce the risk of damaging the fuel assembly during LOCAs, alternative candidate cladding materials are investigated and evaluated with respect to oxidation kinetics above 1000<sup>0</sup>C in a water vapor environment.

Potential candidate materials include austenitic and ferritic/martensitic stainless steel alloys. These samples were prepared with uniform geometry and characterized using a Netzch F3 Simultaneous Thermal Analyzer (STA) equipped with a specialized water vapor furnace. This apparatus can maintain static or dynamic temperature profiles up to 1200<sup>0</sup>C with water vapor content up to 100% for tens to hundreds of hours while continuously reporting the change in mass of the sample. Additionally, the experimental setup includes a mass spectrometer, which is used to measure reaction products and thereby quantify hydrogen evolution and kinetic dependencies. The mechanism of oxidation and the structure of the oxide are studied with standard cross-sectional microscopy using a FEI Inspect F Scanning Electron Microscope equipped with energy dispersive spectroscopy.

The oxidation kinetics of the candidate alloys are determined from the weight gain curves generated by the STA, and are a function of the atmosphere and temperature profile. Combining thermogravimetric analysis, mass spectroscopy, and SEM characterization established a reliable method through which the oxidation performance of various candidate materials may be assessed and evaluated with respect to temperature, environment, and resistance to damage during LOCA conditions.

**Name:** Dylan Rittman  
**Program:** GRA  
**School:** University of Michigan  
**Group:** MST-7  
**Mentor:** Andrew Nelson  
**Category:** Materials Science  
**Type:** Technical Talk  
**LA-UR:** 13-25724

## **Thermophysical Properties of Stoichiometric CeO<sub>2</sub>**

Plutonium is a primary constituent of mixed oxide (MOX) fuel. During burn-up of the fuel, PuO<sub>2</sub> can be formed. In order to accurately model the behavior of MOX fuel in a reactor, it is important to know the thermophysical properties of the oxide phase. However, due to its toxicity, high activity, and proliferation risk, PuO<sub>2</sub> is very costly and difficult to work with. Because of this, CeO<sub>2</sub> is commonly used as a surrogate material due to the hypothesized physical, thermal, and chemical similarities of the two ceramics. Despite this, there is dearth of data in the literature when it comes to the three of the main thermophysical properties of CeO<sub>2</sub>: thermal diffusivity ( $\alpha$ ), heat capacity (CP), and density ( $\rho$ ). In the work presented here, the thermal conductivity ( $\lambda$ ) of stoichiometric CeO<sub>2</sub> was determined experimentally for the first time up to 1500°C. It is known that thermal conductivity is the product of  $\alpha$ , CP, and  $\rho$ . Consequently, temperature-dependent measurements were performed on all three parameters using laser flash analysis (LFA), differential scanning calorimetry (DSC), and dilatometry (DIL), respectively. The results allowed thermal conductivity to be calculated and modeled using the functional form  $\lambda=(A+BT)^{-1}$ . The thermal conductivity of CeO<sub>2</sub> was then compared to that of PuO<sub>2</sub> in order to determine what correction, if any, needs to be taken into account when conducting thermophysical work where CeO<sub>2</sub> is used as a PuO<sub>2</sub> substitute.

**Name:** Brandon Runnels  
**Program:** GRA  
**School:** California Institute of Technology  
**Group:** T-3  
**Mentor:** Irene Beyerlein  
**Category:** Materials Science  
**Type:** Technical Talk  
**LA-UR:** 13-25599

## **Analytical Prediction of Material Interface Energy and Morphology**

In understanding and modeling material energetics, an important factor is the interfacial energy resulting from the mismatch of two crystal lattices. Therefore an accurate and robust model for interfacial energy is useful for modeling mechanical behavior of multi-phase materials, and in understanding and predicting interface stability in the context of multi-material composite design. In this presentation, an approach for understanding and modeling arbitrary interface energy based on Fourier analysis and direct methods in the calculus of variations is developed. Finally, the theoretical results are compared with analytical, computational, and experimental results from literature, and the overall accuracy and robustness of this model is assessed.

Ultimately, this research will enhance the design of strong and lightweight multi-material nanocomposites containing a high density of bimetallic interfaces.

**Name:** Christian Sorensen  
**Program:** UGS  
**School:** New Mexico Institute of Mining and Tech  
**Group:** WX-9  
**Mentor:** David Moore  
**Category:** Materials Science  
**Type:** Technical Talk  
**LA-UR:** 13-25838

## **Explosive Material Response to Acoustics and RF**

The aim of this work is to improve stand-off detection of explosives in the field environment. This presentation covers work looking at the e/m coupling effects to acoustic energy input in several inert and energetic materials, as well as off-frequency response to RF stimulation in these materials. This research will help elucidate the anticipated non-linear response of bulk explosives to GHz & THz EMR.

**Name:** Gillian Hsieh Ratliff  
**Program:** UGS  
**School:** Pitzer College  
**Group:** NEN-3  
**Mentor:** Davis Thomsen  
**Category:** Non-Technical  
**Type:** Non-Technical Talk  
**LA-UR:** 13-25542

## **Global Proliferation: Case Studies of Procurement Attempts**

Aspiring proliferant state and non-state actors' development of weapons of mass destruction (WMD) is a problem the broad majority of nations collectively seek to inhibit. Commercially sold commodities with legitimate civilian uses or even conventional military use can also be of use in the development of WMD. These commodities are protected by adherence to international agreements in the form of implementation of legislation. Illicit procurement networks arise out of the resultant need to circumvent the provisions of this legislation such as End User and End Use verification both on the part of the law enforcement community and the commercial vendors themselves.

In this presentation I will give a brief overview of the proliferation of sensitive goods and present several recent and representative case studies of illicit procurement attempts. These cases illustrate examples of desired commodities, methods of circumventing regulations and commercial best practices, red flags for both law enforcement and commercial enterprise that indicate suspicious transactions, and potential consequences of participation in these networks. Finally, I will present a broader context of my program's role in the prevention and detection of these attempts and its place in the global nonproliferation community.

**Name:** Benjamin Wolkov  
**Program:** UGS  
**School:** Brandeis University  
**Group:** IAT-1  
**Mentor:** Galya Balatsky  
**Category:** Non-Technical  
**Type:** Non-Technical Talk  
**LA-UR:** 13-25139

## **An Insider Threat Analysis of Egypt**

The International Atomic Energy Agency states that every country possessing nuclear material is responsible for the physical protection of it. Yet while the focus of physical security concentrates on external threats such as penetration of facilities by hostile groups, insider threats—acts perpetrated by someone with authorized access to said materials—pose a particularly tricky and understudied problem. Because insiders have access to the materials as part of their job, it is possible for them to steal material, sabotage equipment, and aid outsiders in gaining access to the facilities without raising suspicion. In a 2008 report, the IAEA lays out methods to prevent potential malicious insiders from being hired and how to protect against the case of an insider threat arising. A list of IAEA expectations for protection against insider threats was established using key concepts from the report. Egypt is interested in building civilian nuclear energy while facing many developmental issues, such as an inexperienced workforce, an unstable political and social climate, and low pay coupled with a history of corruption, among other things. Following the establishment of the list of IAEA recommendations, background research was pursued to dissect Egypt's existing facilities and agencies, its intentions for the future, and past cases of security breaches involving nuclear material or facilities. The conclusion is that while Egypt has generally followed IAEA safeguards, its facilities are vulnerable to insider threats because Egypt has insufficient security infrastructure and human capital to ensure their protection. These findings provide guidelines for how to assist and remedy the current security weaknesses to ensure that Egypt is able to execute its activities in a safe, secure and sustainable manner and minimize future risks to its nuclear facilities.

**Name:** Steven Harris  
**Program:** UGS  
**School:** Carnegie Mellon University  
**Group:** P-25  
**Mentor:** Dale Tupa  
**Category:** Physics  
**Type:** Technical Talk  
**LA-UR:** 13-25572

## **A Comparison of Muon Imaging Techniques**

It has been known for several decades that muons created by cosmic ray-induced particle showers can be used to image high Z-number materials. In the past, muon transmission imaging - looking for the number and location of muons that pass through an object - was the common method of muon tomography. However, a team of scientists at Los Alamos National Lab developed muon scattering tomography imaging, a more effective imaging method. By tracking the muon as it enters and as it leaves the sample, one can use the scattering angle to deduce the Z-number of the part of the sample the muon passed through. The Muon Team at LANL developed the Muon Mini-Tracker (MMT) which uses layers of aluminum drift tubes surrounding a sample material to detect incoming and outgoing muons. Recently, a carbon-fiber tube MMT has been developed to fix some of the deficiencies of the aluminum MMT, including the aluminum's interference with the muons and a lack of portability. Currently, the carbon-fiber version of the MMT is collecting data that will be compared to that of the old MMT. Additionally, a model of the new MMT has been developed in Geant4, a Monte Carlo simulation software, so that baseline estimates of its behavior can be obtained.

**Name:** Kevin Huang  
**Program:** GRA  
**School:** University of California- San Diego  
**Group:** MPA-CMMS  
**Mentor:** Marc Janoschek  
**Category:** Physics  
**Type:** Technical Talk  
**LA-UR:** 13-25535

## **Tuning of Strong Electronic Correlations in Actinide Compounds**

The behavior of the 5f electrons of the actinide series changes between two extremes while the 5f electron shell is progressively filled. In the early part of the series, the 5f electrons are itinerant and the dependence of the ionic radius is similar to the transition metals. However, the late actinides (Am and heavier) have large ionic radii resembling the rare earth series, and the 5f electrons are localized. Uranium's position in the actinide series is near to the transition between these two extremes, and therefore U compounds can frequently easily be tuned between them. Notably, Hill has shown that U compounds with small U-U spacing often exist in the itinerant limit that promotes metallic states such as unconventional superconductivity, where as a large U-U distance leads to localized 5f electrons and magnetic ground states. In the intermediate regime where the 5f electrons are neither fully itinerant nor localized, the hybridization of the 5f electrons with the conduction electrons of a material leads to strong electronic correlations, which in turn frequently lead to the emergence of novel states such as non-Fermi-liquid behavior or the hidden order state in  $\text{URu}_2\text{Si}_2$ . Here we have used chemical substitution in high-quality actinide synthesis as a tool to tune the lattice spacing of U compounds, and thus their electronic properties. In particular, we have studied the hidden order compound  $\text{URu}_{2-x}\text{Fe}_x\text{Si}_2$ , where Fe substitution tunes the material between the hidden order state and a neighboring antiferromagnetic phase, as well as  $\text{UCo}_{1-x}\text{Fe}_x\text{Ge}$  and  $\text{U}_4(\text{Ru}_{1-x}\text{Os}_x)_7\text{Ge}_6$  in which chemical substitution suppresses a ferromagnetic phase at a quantum phase transition, where non-Fermi-liquid behavior is observed. We will introduce the material synthesis methods used for these projects, and give an overview of the studied systems and present first results on their properties.

**Name:** Jonathan Lassiter  
**Program:** GRA  
**School:** Alabama A&M University  
**Group:** P-21  
**Mentor:** Chad Olinger  
**Category:** Physics  
**Type:** Technical Talk  
**LA-UR:** 13-25549

## **Modeling of Solar Wind Implantation Profiles Through Use of SRIM**

In 2001 Genesis was launched and remained outside of the magnetosphere at the Sun-Earth L1 Lagrangian point. Here it collected solar wind in four regimes (bulk, coronal mass ejection, interstream, coronal hole). These solar winds are thought to represent the composition of the sun, the external layer of which is believed to have approximately the same composition as the solar nebula from which the solar system was created. To achieve this goal the Genesis probe was fitted with ultra-clean collection materials, optimized for each element of interest. The mission duration was two years, five months and nineteen days. In order to more accurately determine the solar isotopic composition Stopping Range of Ions in Matter (SRIM) simulations were implemented to correct measured fluences for ions that backscattered from the target materials. Due to the hard landing of the spacecraft and associated contamination of collection surfaces, these simulations gained more importance in that they enable function fitting of measured implant profiles at depth that can then be extrapolated into the contaminated shallow regions. These have been taken into account through use of SRIM, and compared to ablated samples from genesis for reference. SRIM uses a Monte Carlo method, with inputs derived from a measured solar wind distribution in each regime for several different elements.

**Name:** Peter Schulze  
**Program:** GRA  
**School:** University of Utah  
**Group:** WX-9  
**Mentor:** David Moore  
**Category:** Physics  
**Type:** Technical Talk  
**LA-UR:** 13-24775

## **Shock Hugoniot Equations of State for Liquid Mixtures**

Laser shock Hugoniot data were obtained using ultrafast dynamic ellipsometry (UDE) for both nonideal (ethanol/water solutions with mole percent  $\chi_{\text{ethanol}} = 0\%, 3.4\%, 5.4\%, 7.5\%, 9.7\%, 11\%, 18\%, 33\%, 56\%, 100\%$ ) and ideal liquid mixtures (toluene/fluorobenzene solutions with mole percent  $\chi_{\text{toluene}} = 0\%, 26.0\%, 49.1\%, 74.9\%, 100\%$ ). The shock and particle velocities obtained from the UDE data were compared to the universal liquid Hugoniot (ULH) and to literature shock (plate impact) data where available. It was found that the water UDE data fit to a ULH-form equation suggests an intercept of 1.32 km/s, lower than the literature ambient sound speed in water of 1.495 km/s (Mijakovic et al. J. Mol. Liq.2011, 164, 66–73). Similarly, the ethanol UDE data fit to a ULH-form equation suggests an intercept of 1.45 km/s, which lies above the literature ambient sound speed in ethanol of 1.14 km/s. Both the literature plate impact and UDE Hugoniot data lie below the ULH for water. Likewise, the literature plate impact and UDE Hugoniot data lie above the ULH for ethanol. The UDE Hugoniot data for the mixtures of water and ethanol cross the predictions of the ULH near the same concentration where the sound speed reaches a maximum. In contrast, the UDE data from the ideal liquids and their mixtures are well behaved and agree with ULH predictions across the concentration range. The deviations of the nonideal ethanol/water data from the ULH suggest that complex hydrogen bonding networks in ethanol/water mixtures alter the compressibility of the mixture.

**Name:** Robert Zedric  
**Program:** GRA  
**School:** Texas A&M University  
**Group:** NEN-1  
**Mentor:** Daniela Henzlova  
**Category:** Physics  
**Type:** Technical Talk  
**LA-UR:** 13-25631

## **Modeling an Active-Interrogation Device for Spent Nuclear Fuel Measurements**

The International Atomic Energy Agency (IAEA) makes the world a safer place by applying safeguards to civilian nuclear materials. This helps deter non-nuclear weapons states from diverting civilian materials to covert nuclear weapons programs. The IAEA regularly monitors nuclear material inventory in civilian facilities to detect theft in a timely manner. Keeping accurate inventory of plutonium content in spent nuclear fuel presents a difficult challenge. Californium-Interrogation with Prompt Neutron detection (CIPN) is a new concept being developed to address this. It incorporates four neutron and two gamma-ray detectors in a compact case that can be lowered deep into a spent fuel pool. A capsule of neutron-emitting californium-252 is placed near the fuel assembly to induce fissions. Background readings are subtracted from the active-interrogation measurement to analyze the fissile material content. Monte Carlo N-Particle transport code (MCNPX) is used to characterize the CIPN behavior over a range of spent fuel assemblies. These simulations help correlate the detector response to the initial U-235 enrichment, irradiation history, and post-irradiation cooling time for each assembly. The Korea Atomic Energy Research Institute (KAERI) will host prototype testing with seven Korean spent fuel assemblies in October 2013.