Los Alamos National Laboratory

"Championing Scientific Careers"
Highlighting Student Research

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2014 Student Symposium

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Student Last Name	Student First Name	Title	Category
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Jakhar	Shailja	Integrative Bio Surveillance	Biosciences
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Sward	Jeffrey	Using a Microfluidic Approach to Analyze Bacteria Growth and Antibiotic Response	Biosciences
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Macor	Joseph	Selective Extraction of Minor Actinides with Heterocyclic Dithiophosphinic Acids	Chemistry
Hendon	Raymond	Conduction Invariance in Exact Solutions for Compressible Flow Code Verification	Computing
Schenker	Arley	Computer Vision Algorithms for Labeling Social Media Video	Computing
Turrubiates	Benjamin	Auto-Generated ClusterWide Configuration Tool	Computing
Biaou	Carlos	Improving Modeling of Solar Wind Ion Implantation	Earth and Space Science

Dolan	Sean	Obsidian Procurement and Social Interaction on the Pajarito Plateau A.D. 1200-1600	Earth and Space Science
Boardman	Beth	Optimal Kinodynamic Motion Planning in Environments with Unexpected Obstacles	Engineering
Clark	Kimberly	Characterization of the NPOD3 Detectors in MCNP5 and MCNP6	Engineering
Kerby	Leslie	Intermediate-Energy (> 1 MeV) Cross Section Models in CEM and MCNP6	Engineering
Madsen	Jonathan	Shared Memory Parallelism of MCATK with Minimal Locking Synchronization	Engineering
McKenzie	George	Rossi Alpha Method	Engineering
Miles	Lillian	Modeling Quasielastic Release	Engineering
Papp	Joseph	Gas Transport Characterization of Elastomeric Sealant Materials	Engineering
Swift	Alicia	Verification of the MCNP6 FMESH Tally	Engineering
Crawford	Jesse	Infrastructure Automation with Puppet	Information Technology
L'Esperance	Nathan	ADPSM Document Control and Resumption Process Revisions	Information Technology
Cherukara	Mathew	Shock Induced Chemistry in Granular Ni/Al Reactive Intermetallics	Materials Science
Hahn	Eric	Physics of High Strain Rate Damage: NEMD Simulation Studies	Materials Science
Reynolds	Jonathan	Characterization of Sensor Response as a Function of Electrode Composition	Materials Science
Sooby	Elizabeth	Ion Beam Experiment to Simulate Simultaneous Salt Corrosion and Neutron Damage	Materials Science
Stewart	Anthony	Probing the Electrochemical Characteristics of Aged Carbon-Supported Pt Catalysts	Materials Science
Hughes	Heather	Sociocultural Dimensions of Literacy/Biliteracy Development	Non-Technical --Education
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Jaffke	Patrick	New Algorithms to Verify Declared Reactor Operations Via Fission Product Isotopics	Physics
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Melvin	Jeremy	Evolution of Rayleigh-Taylor Growth After an Initial Richtmyer-Meshkov Instability	Physics
Morgan	Taylor	Core Convection, a Driving Mechanism for Gamma Doradus – Delta Scuti Pulsations	Physics
Runnels	Brandon	A New Model for Interface Energy	Physics

Shields	Daniel	SPIDER Progress Towards High Resolution Correlated Fission Product Data	Physics
Wood	Mitchell	Molecular Dynamics Simulations of Chemistry Induced by Void Collapse in RDX	Physics

Name: Esteban Abeyta
Program: HS COOP
School: Los Alamos High School

Name: Ashvini Vaidya
Program: HS COOP
School: Los Alamos High School

Group(s): DSA-03, MPA-CINT
Mentor: Alina Deshpande, Kristin Omberg
Category: Biosciences
Type: Group Poster Presentation
LA-UR: 14-25118

Presymptomatic Detection of Disease

The mixture of organisms naturally found on surface tissues is referred to as natural flora. The composition of natural flora of gut, skin and other surfaces of the body can be influenced by a large range of factors. Humans need specific microbes to maintain health. Microbial composition of the natural flora could serve as an indicator of health or disease. Detection of disease within the human body is based upon symptoms an individual may experience. If our hypothesis were supported, a test could be developed in which oral samples could be analyzed to determine the health status of an individual before symptoms. To test our hypothesis, that changes in the normal flora of yogurt can indicate whether the yogurt is normal or spoiled as a model for health and disease state and thus changes in the normal flora of the human mouth can be indicators of health and disease status, we used procedures that included bacterial plating, polymerase chain reaction, gel electrophoresis, and sequence analysis using bioinformatics. The work presented in this study are the first step and second step in confirming our hypothesis that we will be able to monitor natural flora in a way that allows us to determine whether oral flora can be an indicator of health. We have mastered basic microbiology and molecular biology techniques to continue our study and reach our goal of creating a diagnostic test that would allow us to see if a human being will become sick by any changes in the composition of the oral microbiome.

Name: Kirill Balatsky
Program: GRA
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Group: B-11
Mentor: Pete Silks
Category: Biosciences
Type: Individual Poster Presentation
LA-UR: 14-25538

Heavy Atom Substituted Tryptophan Analogs and Three Dimensional Imaging

Synthesis of Te and Se substituted tryptophan (an essential amino acid), analogs for three dimensional protein imaging (through NMR spectroscopy, Mass spec, and X-ray crystallography) can help solve the phase problem inherent in protein imaging. Tryptophan is an ideal amino acid to synthesize and use for this task because of its tendency to be incorporated inside most proteins and the added heavy atom in this molecular architecture could help improve the results of scattering X-Rays better for crystallography studies or for use in NMR.

The synthesis begins with a commerically available tosyl pyrrole. Metallation of the C2 carbon followed by adding elemental selenium effects insertion into the carbon lithium bond giving rise to a selenide anion. Alkylation with an acetaldehyde surrogate affords the derivatized pyrrole in 80-90% purified yields. In one contiguous series of chemical steps the C2 atom of the pyrrole is oxidized under basic conditions and the pre-cyclization side chain is installed. Polyene cyclizations are well known, with W. S. Johnson (Stanford University) installing molecular elements which provided for good initiation and termination methods. The next step is a single "polyene" cyclization. Treatment of the selenide with a Lewis acid cleanly effects the cyclization and aromatization in one step. The resulting product is a selenophene pyrrole, an indole analog with a tosyl protecting group that is all that remains to be removed. Methoxide cleaves this group off. Enzymatic coupling of serine by tryptophan synthase completes the synthesis of the "mutant" amino acid for use in the expression of an inducible protein.

Name: Miranda Barraza
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Group: B-10
Mentor: Jean Challacombe
Category: Biosciences
Type: Individual Poster Presentation
LA-UR: 14-25517

Antibiotic Resistance in Francisella Species

Francisella tularensis is a gram-negative, bacterial pathogen that causes the disease tularemia in both humans and animals. F. tularensis subspecies tularensis, also known as Type A, is endemic in North America and causes a severe form of tularemia, while F. tularensis subsp. holarctica, or Type B, is primarily found in Europe and Asia and causes a milder form of the disease. Other species, such as F. tularensis subsp. novicida, are naturally found in the environment, but can cause disease in immune compromised hosts. Depending on the route of transmission, symptoms may involve a combination of skin lesions, swollen lymph nodes, fever, or pneumonia. Tularemia can be acquired by direct contact with infected animals, arthropod bites, oral consumption of contaminated water or food, or by inhalation of an aerosolized form of the bacteria. This last method of transmission is of great concern regarding bioterrorism, because respiratory transmission of Type A F. tularensis causes acute onset of pneumonia-like symptoms, which may prove fatal without antibiotic treatment.

A number of antibiotics are successful in treating tularemia, but F. tularensis has already proven its ability to become resistant to beta-lactam antibiotics, erythromycin, and to co-trimoxazole, or sulfamethoxazole/trimethoprim1. In this study, we compared the genome sequences of thirty Francisella strains, including strains of F. philomiragia, an opportunistic pathogen also present free-living in the environment, and F. noatunensis, which causes disease in fish, to determine which genomes contained certain antibiotic resistance genes. We specifically focused on the bla1 and bla2 genes, which encode beta-lactamase enzymes (inactivators of beta-lactam antibiotics)2. Further comparisons of efflux pump genes and additional antibiotic resistance mechanisms found in the environmental Francisella species are in progress.

1. Silpak Biswas, Didier Raoult, Jean-Marc Rolain. A bioinformatic approach to understanding antibiotic resistance in intracellular bacteria through whole genome analysis. International Journal of Antimicrobial Agents 32 (2008) 207–220.
2. Bina XR, Wang C, Miller MA, Bina JE. The Bla2 beta-lactamase from the live-vaccine strain of Francisella tularensis encodes a functional protein that is only active against penicillin-class beta-lactam antibiotics. Arch Microbiol. 2006 Sep;186(3):219-28. Epub 2006 Jul 14.

Name: Celeste Bean
Program: UGS
School: University of California, Santa Barbara
Group: T-6
Mentor: Sandrasegaram Gnanakaran
Category: Biosciences
Type: Individual Poster Presentation
LA-UR: 14-25614

Automated Data-driven Modeling of Multi-drug Resistant Efflux Pumps

Bacteria's increasing resistance to antibiotic treatments necessitates a comprehensive understanding of the means by which pathogens reject toxic agents. Multi-drug resistance (MDR) efflux pumps are proteinaceous molecular machines that recognize a wide array of antibiotics and drugs, change conformation, and export agents from the cell. Our current techniques for modeling the efflux pumps iteratively use experimental data from homologous proteins--proteins with a shared ancestor--to corroborate computational predictions, but the protocol requires trained, manual intervention at each stage. We broaden our approach by fully automating the modeling process to produce data-driven atomic models of uncrystallized MDR efflux pumps with the goal of developing more effective pharmaceutical techniques for circumventing the pumps' drug resistance.

Name: Amanda Mercer
Program: UGS
School: Whitman College
Group: B-10
Mentor: Jean Challacombe
Category: Biosciences
Type: Individual Poster Presentation
LA-UR: 14-25548

Antibiotic Resistance Genes in Burkholderia Pseudomallei

Burkholderia pseudomallei is a Gram-negative bacterium that causes the disease melioidosis in humans. Melioidosis is endemic in Southeast Asia, Northern Australia, Africa, the Middle East, and South America. B. pseudomallei is an environmental saprophyte found in wet soils and standing water. It is a potential biothreat agent due to its ability to infect humans through inhalation of contaminated dust or water droplets, ingestion of contaminated water, and contact with contaminated soil and water. A related species, Burkholderia mallei, causes the disease Glanders in horses. B. pseudomallei is intrinsically resistant to a large number of antibiotics, whereas B. mallei is generally more sensitive to antibiotics. Neither bacterium has a current vaccine available.

For this project, we investigated antibiotic resistance mechanisms in B. pseudomallei and B. mallei using comparative genomics methods. Some of the main antibiotic resistance mechanisms in B. pseudomallei are its efflux pumps2. Another mechanism used by the Burkholderias is β-lactamase1. Efflux pumps are proteinaceous transporters located in the bacterial cell membrane. The efflux pumps that assist in antibiotic resistance are AmrAB–OprA, BpeAB–OprB, and BpeEF–OprC. AmrAB–OprA is responsible for resistance to acriflavine, aminoglycoside, and macrolide antibiotics. BpeAB–OprB contributes to acriflavine resistance. BpeEF–OprC contributes to resistance to chloramphenicol, fluoroquinolones, tetracyclines, trimethoprim, and co-trimoxazole.

Through genomic comparisons, we determined that the amrAB–oprA operon was present in several B. pseudomallei genomes, but was present in the B. mallei SAVP1 genome. However, B. mallei SAVP1 lacked the genes comprising the bpeEF–oprC operon. All of the B. pseudomallei genomes contained the Class Dβ-lactamase gene, which provides resistance against cloxacillin and penicillin. The Class Dβ-lactamase gene was absent from all B. mallei genomes tested. However, genes encoding the BpeAB–OprB efflux pump and Class Aβ-lactamase were found in all of the genomes that we examined.

1. Niumsup, Pannika and Vanaporn Wuthiekanun. “Cloning of the Class D β-lactamase Gene from Burkholderia pseudomallei and Studies on its Expression in Ceftazidime-susceptible and -resistant Strains.” Journal of Antimicrobial Chemotherapy. 2002, 50, 445–455.
2. Schweizer, HP. “Mechanisms of Antibiotic Resistance in Burkholderia pseudomallei: Implications for Treatment of Melioidosis.” Future Microbiol. 2012, 7, 1389-99.

Name: Juliette Ohan
Program: UGS
School: California State University, Los Angeles
Group: B-11
Mentor: Shawn Starkenburg
Category: Biosciences
Type: Individual Poster Presentation
LA-UR: 13-23496

Interrogation of Interspecies Relationships in Algal Production Cultures

A growing body of literature suggests that many unicellular algae (microalgae) require bacteria to provide essential nutrients and metabolites for optimal growth and survival in natural microbial ecosystems. Unfortunately, the scientific community has little knowledge regarding the extant bacterial mediated effects on algal nutrient utilization or growth. These same unicellular microalgae have been targeted for commercial applications because of their ability to efficiently accumulate biomass and/or lipids for conversion into renewable transportation fuels and other useful bioproducts. Research conducted to improve the productivity of commercial algal ponds has relied on the extrapolation of growth studies conducted under axenic laboratory conditions and have neglected to consider the positive (or negative) impact of bacteria. To discover and identify these algal-bacterial interactions, we are developing a methodology to efficiently capture a small quantity of bacterial cells in porous agarose beads (gel microdroplets or 'GMDs') for cultivation with the algae in a microfluidics chamber. In parallel, we have developed a workflow to monitor growth within these GMDs and subsequently recover cells with the desired phenotypes. When realized, our goal is to determine which bacteria modify algal physiology to increase biomass yield and/or reduce nutrient input to immediately impact the productivity of algal biofuel production strains. Herein we present progress made towards constructing this culturing system, monitoring bacterial loads in the test cultures, and demonstrate growth of algae within picoliter sized GMDs.

Name: Nicholas Thoma
Program: UGS
School: Iowa State University
Group: B-11
Mentor: Srinivas Iyer
Category: Biosciences
Type: Individual Poster Presentation
LA-UR: 14-25534

MALDI Mass Spectrometry of Explosive Compounds

Typical analysis of explosives utilizes Gas or Liquid Chromatography (GC or LC) methods. However, high-nitrogen small molecule explosives readily decompose in the GC process, and salts are unobservable by LC. Therefore, alternative methods are needed to analyze these types of molecules. An exceptional alternative to GC or LC is MALDI-MS (Matrix Assisted Laser Desorption Ionization-Mass Spectrometry). Commercial matrices like Alpha-cyano-4-hydroxycinnamic acid (αCHCA) or 2,5-dihydroxybenzoic acid (2,5-DHB) are used in peptide and small molecule analysis, and themselves readily ionize. Our MALDI-MS (and most other commercially available) instrument is equipped with a 337nm wavelength nitrogen laser. αCHCA and 2,5-DHB absorb strongly at 337nm and have chemical structures incorporating conjugated double bonds; these are attributes most commonly associated with rapid and efficient absorption of laser irradiation.

In this pilot project, our focus is two-fold: i) Develop MALDI-MS methods to analyze high-nitrogen small molecules as an alternative to GC or LC methods; ii) Interrogate a suite of small molecule explosives and determine if they possess potential to serve as matrices for difficult-to-ionize compounds. Preliminary results indicate that some of the tested compounds ionize independently with conventional matrices. There were a few compounds that would not ionize in either mode; we are investigating appropriate methods to analyze these compounds. A library of > 400 molecules are available to us for analysis. Based on our initial results, we will screen and down select a subset of these molecules and examine the effect of conjugated bonds and absorbance at about 337nm on ionization potential.

Name: Anais Weibel
Program: GRA
School: University of Paris Diderot
Group: B-11
Mentor: Momo Vuyisich
Category: Biosciences
Type: Individual Poster Presentation
LA-UR: 14-25463

In Vitro Evolution of Influenza a Virus Under Artificial Selective Pressure

RNA viruses cause many significant diseases worldwide, such as Dengue and Yellow fevers, the Flu, AIDS, etc. These viruses evolve rapidly and few antiviral therapeutics and vaccines exist. Viral evolution remains poorly understood.

We are studying the evolution of RNA viruses under laboratory conditions. Our research aims to answer important questions about the prediction of virus phenotype from its genotype, protein mutations and function, and functions of structural RNAs. We are currently focused on the human Influenza A virus (IAV).

Our experimental design creates an artificial environment for viral infection and our hypothesis is that we will be able to direct the viral evolution in a specific and desired way. We have engineered host cells (supplemented cells) to express proteins that the IAV naturally produces. After a series of infections of the supplemented cells, we will study the effect of this supplementation on the viral evolution. We expect that the viral population will evolve to efficiency infect the supplemental cells and lose the ability to infect the wild-type (natural) cells. If our hypothesis is correct, this approach may provide novel viral therapeutic approaches.

Name: Sarah Bouquin
Program: HS COOP
School: Los Alamos High School
Group: MPA-CINT
Mentor: Jennifer Hollingsworth
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25363

Monitoring the Nanocrystal-to-Supercrystal Transformation In Situ and Real-Time

We use electrostatic assembly of oppositely charged nanocrystals to synthesize "supercrystals." Supercrystals are ordered three-dimensional assemblies of nanocrystals that resemble conventional crystals in the periodic arrangement of the component nanocrystals. As crystals are made up of atoms, supercrystals comprise nanocrystals, which are often referred to as "artificial atoms." When solutions of positively and negatively charged nanocrystals are mixed, attractive electrostatic interactions cause the particles to assemble. If the attractive forces are too strong, the resulting assembly is disordered, or "amorphous." Conversely, if too weak, the nanocrystals will not assemble at all, remaining separate and suspended in their solvent. Under certain conditions, however, the attractive forces promote ideal, controlled nanocrystal assembly and formation of ordered supercrystals. Here, we investigate factors that can influence the strength of the nanocrystal interactions: magnitude of nanocrystal surface charge (tuned by changing the pH of the solution), electrolyte concentration (or other additives that can be used to partially "screen" nanocrystal surface charge), nanocrystal concentrations, and nanocrystal size distributions. We apply a unique technique to "see" in situ and real-time the nucleation and growth of the nanocrystal assemblies from small clusters of only a few nanocrystals to larger micron-sized supercrystals. We use a NanoSight microscope fitted with a camera to capture videos of our nanocrystals suspended in water. Through the instrument's Nanoparticle Tracking Analysis software, we can determine the average size and size distribution of the nanocrystals in real-time as they assemble into clusters and even larger assemblies. Thereby, we can directly determine the impact of our experimental variables on the rate of nanocrystal assembly, giving us the ability to control and optimize the process of supercrystal growth.

Name: Ty Brooks
Program: UGS
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Group: C-IIAC
Mentor: Andy Sutton
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25631

Understanding Biomass Derived Transportation Fuels

As the world's dependency on petrochemical derived transportation fuels continues to grow there is an increasing effort to research renewable energy alternatives. Biomass derived fuels are an attractive alternative to fossil fuels due to the fact that they can utilize the current infrastructure for transportation fuels. It has been shown that cellulose and hemicellulose biomass can be transformed into platform chemicals like furfural and 5-hydroxymethylfurfural. These platform chemicals can in turn be transformed into linear polyketone carbon chains. The next step in the process is to cleave the oxygen bonds to create linear alkane carbon chains for use as drop in ready transportation fuels. This is done through a hydrodeoxygenation (HDO) reaction, and is the most energy intensive process in the conversion of biomass to fuel. The model compounds 3-pentanone and 2,5-hexanedione were used to form better knowledge of this HDO process and the intermediate molecules formed along the way. Understanding the stepwise process will lead to identifying the most energy intensive steps in these HDO reactions. Focus can then be put into finding better catalysts to reduce the overall energy input for alkane synthesis.

Name: Jamie Daum
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Group: C-NR
Mentor: Evelyn Bond
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25452

Determination of Radioisotopes in Post-Detonation Scenarios

Nuclear Forensics is the analytical characterization and evaluation of nuclear materials that are either intercepted in a pre-detonation state or retrieved from post-detonation debris and fallout. The characterization and evaluation conducted on the confiscated nuclear forensic evidence allows law enforcement and intelligence agencies to prevent, mitigate, and attribute radiological or nuclear incidents. Post-detonation debris contains trace-level quantities of nuclear material along with materials found within the environment of the detonation site. Post-detonation forensics requires innovative radioanalytical techniques in order to isolate, characterize, and determine the nuclear material within the debris. Radioanalytical techniques have been widely used to determine radioisotopes within a variety of matrices. Post-detonation debris, however, contains a variety of matrix constituents that could inhibit these techniques. Modern radioanalytical separation techniques employ novel extraction chromatographic resins in order to separate radionuclides from sample matrices. The research employs novel extraction chromatographic resins in order to determine the effect of matrix constituents, such as those found within post-detonation debris and fallout, on their retention capabilities for the radioisotopes of interest. Batch experiments were conducted in order to determine the effect of salt matrix constituents on their retention capabilities for the radioisotopes of interest, particularly isotopes of plutonium. The extraction chromatographic resins that were being analyzed within this experiment were commercially available resins manufactured by Eichrom Technologies, LLC which included: UTEVA® Resin, TEVA® Resin, TRU Resin, and DGA Resin. The selective extraction of the radioisotope of interest was followed by liquid scintillation counting (LSC) to determine the retention capability of the resin. The retention capabilities of the resins were measured by the capacity factor, k', which is the free column volumes to peak maximum. The greater the value of the capacity factor, the more affinity the resin had for the radioisotope of interest.

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Mentor: George Goff
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25684

Investigation of Ionic Liquids for Electrochemical Separations of Uranium

In recent years ionic liquids (ILs) have garnered attention as they have been shown to be advantageous compared to aqueous and other organic environments in various ways including low volatility and high stability. Both actinides and lanthanides are extremely electropositive and typically require rather large reduction potentials which cannot be accessed in aqueous solution without competing solvent reactions. However, sufficiently negative potentials are achievable in certain ILs. These broader potential windows provided by ILs can be capitalized upon for the reduction of f-elements. The ultimate goal is to separate a single component by deposition from a mixture of actinide and lanthanide species in IL.

The goal of the summer project was to investigate three ionic liquids (ILs) containing the bis(trifluoromethanesulfonyl)imide anion in regards to electrodeposition of Nd and U, especially as a mixed sample. What separation of U from Nd could be achieved?
UV-Vis spectroscopy was used following extraction of the U and Nd from IL samples by contacting with 1 M HClO4 to determine the initial ratio of U:Nd in the IL samples. Cyclic voltammetry was performed at elevated temperature and potentiostatic electrodepositions were then conducted on the IL samples at various negative potentials using a Cu foil working electrode. Deposits obtained were cleaned, dried, and then dissolved in 1 M HClO4 for UV-Vis analysis of the resulting U/Nd ratio.

Preliminary results incidate Nd does not easily electrodeposit and only minimal deposit was obtained. With respect for separations from a mixed U/Nd sample in the ILs, spectroscopy of dissolved deposits indicated separation has occurred due to decreased presence of Nd compared to the U. Additionally, the more positive the electrodeposition potential the better the separation will likely be in the subsequent deposit. Further repeated experiments and optimization of conditions are underway to see the reproducibility of the separation.

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Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25323

Complexes for Stable Chelation of Actinium and Actinium-Daughter Radioisotopes

Radionuclides are commonly used for biological imaging and therapy. Gamma-emitters and positron-emitters are favorable for imaging purposes, whereas beta-emitters may be used for therapeutic applications.

Recently, significant research efforts have explored targeted alpha therapy (TAT) as a promising treatment for cancers and infectious disease. Alpha particles properties (i.e., high linear energy transfer and short range) are valuable because they deliver high cytotoxic radiation dose to targeted cells, while limiting damage to non-diseased cells. To assure that the radionuclide is delivered to the desired site in the body, two components are needed: a biological targeting vector and a chelating agent attached to the chosen radionuclide.
A relatively new radionuclide, Ac-225, is lately of interest for TAT. Ac-225 is an alpha-emitting nuclide with a 9.9 days half-life. From the Ac-225 decay scheme, the four alphas emitted come from Ac-225, Fr-221, At-217 and either Bi-213 or Po-213. Alternatively, Ac-225 can be used as a generator for the shorter-lived daughter isotope: Bi-213.

The stability of actinium and bismuth complexes for a series of nitrogen containing heterocycles was investigated. The affinity of the ligands for one or the other metal was investigated as well as the stability of the complexes formed. The labelled complexes were challenged by addition of competing metal ions, or competing ligand such as EDTA. The kinetics of formation of the complexes and their stability were followed by spotting aliquots on a TLC plate. The TLC plates were analyzed using phosphorimaging techniques and gamma spectroscopy. New, viable chelators for Ac-225 and Bi-213 were studied and showed rapid kinetics and elevated stability against various metal ions and ligands that could compete in biological environment.

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Group: C-NR
Mentor: Marianne Wilkerson
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25601

SEM Imaging in Nuclear Forensics

In this project, I began to gather images and sort them using a decision chart devised to classify images based on the particles nature, distribution, and morphology. This was later implemented into a program to go alongside the Genie program in order to make the process of defining the images easier. After the initial visual processing I began to train the Genie program to classify images on its own based on the characteristics found on the decision chart.

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Group: C-IIAC
Mentor: Andrew Sutton
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25628

Development of Catalysts for Coupling Reactions of Relevance to Energy Production

Glycerol, a major by-product of biodiesel production, is inexpensive and abundant. Currently, the usage of glycerol is limited to food stuffs, pharmaceuticals, and some chemical applications such as the conversion into propanediol, acrolein, and polyethers. This research focuses on the conversion of this three-carbon species into higher-value six-carbon compounds that can be utilized as both fuels and feedstocks. The redox-active ligands, which are capable of supporting multiple oxidation states that would otherwise be energetically inaccessible, bond with divalent iron compounds and then undergo a reductive Pinacol coupling process, followed by reaction with a strong acid to release the desired product.

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Mentor: Chris Leibman
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25584

Ammonium Bifluoride Dissolution of Glass Samples for Actinide Assay

Existing methods used to process glassy samples from post-detonation debris use large quantities of concentrated mineral acid and can take up to 7 days to complete. A new approach being considered involves the use of ammonium bifluoride (NH4)HF2 as a dissolving agent for fused glass samples. The use of ammonium bifluoride (ABF) is expected to decrease digestion time to >2 hours and be significantly safer. Initial modeling was performed in order to 1) Determine the necessary parameters for the reactions involving ABF and 2) To apply the parameters to future experiments for the purpose concentrating actinides and determining isotope ratios. OLI Systems software was used to model the solubilities of fluorinated complexes in a HNO3/Al(NO3)3 solution and to determine the concentrations of HNO3 and Al(NO3)3 necessary for sample cleanup and actinide concentration.

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Name: Wade Spurlock
Program: GRA
School: Stanford University

Group(s): XCP-4
Mentor: Daniel Israel
Category: Physics
Type: Group Poster Presentation
LA-UR: 14-25879

Integral Method and Eigenspace Decomposition for Turbulent Mixing Flows

An integral method for RANS turbulent mixing is compared to full-field RANS simulations in the xRAGE code. Eigenspace decomposition reveals dominant solution coefficients and is used to visualize a reduced dimension of parameters. Results are shown for the temporal shear layer, while work is continuing on the Rayleigh-Taylor layer and strong jet.

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Mentor: Andrew Gaunt
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25343

Studies of Actinide Chalcogenide Bonding

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

Name: Rebecca Springs
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Group: C-NR
Mentor: Evelyn Bond
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25576

Methods for Making Ultra-Thin Scintillator Detectors

Ultra-thin scintillator detectors, with scintillator films less than 100 micrometers, are of interest for multiple projects within the nuclear and radiochemistry group at Los Alamos National Laboratory. Ultra-thin scintillator films can be used in detectors to take advantage of the restrictions they place on energies that are seen by the detector. The polyvinyltoluene based EJ-296 scintillator paint will be used. Variations of two different methods will be tested to see which produces the thinnest and most uniform scintillator films. The first method tested will be spin coating the scintillator paint onto a Mylar backing. The second method is water dispersion. Many factors that can have an impact on the final thickness of the scintillator film will be varied in this experiment. The solvent used to dilute the scintillator paint as well as how diluted the paint is play a big role. A solvent with a high vapor point will evaporate too easily, causing the paint to dry too quickly before it can become even and thin. The extent to which the paint is diluted with solvent impacts the viscosity of the paint solution and how thin the final film can be made. Finally, the speed at which the spin coater is spun, or with which you hand pull the film in water dispersion will also change the thickness; faster speeds lead to thinner films. In addition, uneven speeds will give non-uniform films. It is expected that the spin coating method will produce more even films because there is less human error introduced into the experiment. We are hopeful that we can make films as low as 30 micrometers that are even over a 30 centimeter diameter.

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Group: C-NR
Mentor: Marianne Wilkerson
Category: Chemistry
Type: Individual Poster Presentation
LA-UR: 14-25606

Luminescence Studies of Uranyl Compounds in the Solid State

Fluorescence Spectroscopy has been used to detect environmental uranium signatures, both as uranium containing minerals and ores, and as environmental contamination around nuclear sites. Fluorescence Spectroscopy shows potential for use in nuclear forensics as a means of non-destructive analysis of the chemical environment of interdicted uranium materials. The quantum efficiency of uranyl compounds is quite high, with some compounds approaching unity. This fact makes fluorescence spectroscopy of uranyl a prime candidate for forensic applications. Fluorescence Spectroscopy is the process of using photons to excite the electrons of an atom or molecule, and measuring the photon emission as the atom or molecule de-excites. Uranyl compounds show a characteristic emission in the 450-600 nm range, when excited by light in the UV to short-Visible range. The luminescence of the uranyl ion is phosphorescent in character arising from the excitation from the σu U-O bonding orbital to the non-bonding f-type φu orbital, resulting in a 3Δg triplet state. The excitation and emission spectra of several solid uranyl compounds will be recorded. The solid uranyl compounds to be analyzed are uranyl sulfate (UO2SO4), uranyl acetate (UO2(CH3COO)2), uranyl nitrate (UO2(NO3)2), and uranyl fluoride (UO2F2). The compounds were chosen due to their interest for nuclear forensics arising from use in uranium ore concentration and processing, uranium enrichment procedures, or spent nuclear fuel reprocessing. The structure and hydration of each compound will be determined using powder X-ray Diffraction techniques and Fourier-Transform Infrared Spectroscopy.

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Group: HPC-5
Mentor: Michael Lanf
Category: Computing
Type: Individual Poster Presentation
LA-UR: 14-25732

The use of MYSQL as a database backend for MDHIM, a parallel key/value storage mid

Today's software applications designed for cluster and supercomputers produce. However, what if you wanted to look for the next or previous data or have a different database that you want to use. The task becomes increasingly difficult for many key/value store systems. Moreover, it becomes difficult to attempt these operations while taking advantage of high speed networks such as Cray's Gemini and Infiniband. Multi-Dimensional Hashing Indexing MiddleWare (MDHIM) uses C and the Message Passage Interface (MPI). It attempts to solve this issue by doing the following:

Distribute the data to nodes to avoid overloading servers with requests
Make multiple parallel requests
Allow requests that pull the following or previous data
Have multiple database backends to use

Furthermore, using MYSQL expands on some of the features for MDHIM to make it a parallel database key/value storage system.

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Category: Computing
Type: Individual Poster Presentations
LA-UR: 14-25587

Computing Behind the Red Line: Capturing the Legacy

For over 70 years Los Alamos National Laboratory has had unusual prominence at the forefront of high-performance computing (HPC). LANL's history intersects integrally with the birth of the computing industry. Its mission needs drove the early development of high performance computing for the nation and internationally. This notable record of achievement prompted a preliminary survey of LANL's HPC history in 2013, which resulted in heightened awareness of this significant legacy, greater attention to the existing (and potential) historical sources, and a timeline platform to help disseminate this knowledge.

The LANL-HPC History Project was initiated to capture and document both the ordinary and the extraordinary accomplishments that created this history, both technical and non-technical and in the context of the larger (industrial and political) historical backdrop. In 2014, with the support of the Advanced Simulation and Computing (ASC) Program, LANL initiated a multi-year research collaboration with the Charles Babbage Institute and the Department of the History of Science, Technology, and Medicine at the University of Minnesota. Ongoing HPC History Project activities include surveying archival materials at LANL, conducting a set of oral history interviews, developing an interactive framework to make photographs and other historical materials available to staff, and preparation of scholarly articles to be published in the open literature to augment existing sources such as Nicholas Metropolis, et al., A History of Computing in the Twentieth Century: A Collection of Papers (New York: Academic Press, 1980) and Donald MacKenzie's "The Influence of the Los Alamos and Livermore National Laboratories on the Development of Supercomputing" in IEEE Annals of the History of Computing (April-June 1991).

Name: Peter de Vietien
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Group: XCP-4
Mentor: Nathaniel Morgan
Category: Computing
Type: Individual Poster Presentation
LA-UR: 14-25751

Applying a Lagrangian Algorithm to Inertially Confined Fusion Applications

In this work a staggered grid Lagrangian hydrodynamic method, the MARS method was used to simulate the compression of an ICF pellet from the OMEGA facility. The method was tested for its accuracy, its numerical robustness, and its ability to preserve key physical features such as boundary surface instabilities. Experimental data from the OMEGA facility was then used as an input, and the simulation was run using the experimental data. In this work, it was shown that the MARS method is accurate, that its numerical method is more robust than previous methods used for the pressure ball problem, and that small perturbations were preserved and instabilities grew as expected on the material interface surface. This sufficed to justify investigation of the problem using experimental data, the conclusions from which have yet to be drawn.

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Group(s): XCP-4
Mentor: Davis Herring
Category: Computing
Type: Group Poster Presentation
LA-UR: 14-25775

Algorithms for Boundary Coalescence during Mesh Generation

To ensure correct connectivity in a conformal mesh all part-part boundaries must be identified. Currently it is entirely the user's responsibility to correctly identify all part boundaries. Because there may be numerous interfaces, an algorithm for finding 2D part boundary concurrencies has been developed which can automate this process. It is built on mathematical definitions for shared interfaces using a minimal set of numerical tolerances. We have demonstrated that the algorithm produces expected results in a variety of cases. From the outputs of this algorithm, it is possible to build a topological graph that can be used to perform constructive solid geometry (CSG) operations on closed contours while preserving the topological information.

Name: Jeremy Harrod
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Group: EES-16
Mentor: Terry Miller
Category: Computing
Type: Individual Poster Presentation
LA-UR: 14-25665

Discrete Fracture Network Workflow Verification for Public Distribution

Discrete Fracture Network (DFN) modeling is an important approach for simulating subsurface flow and transport in impermeable rocks such as granite, where fractures provide the main pathways for flow and solute transport. We have recently developed a three-dimensional DFN generator model with high-quality computational meshing to simulate accurate flow and particle tracking on large-scale domains. This generator has the capability to reproduce DFNs similar to natural sites. As a result, the model has a wide variety of geological applications, such as modeling of radionuclide contaminants transport and natural gas production.

In order to distribute the DFN workflow to the public and make it available for use to all with interest, a set of verification tests must be performed and new user interface implemented. Testing and code examinations for producing large DFN models leads to the need to manage memory efficiently. Since the program is designed to give the user complete control and has no limitations on the size of model that can be produced, the computer hardware will be the limiting factor. Effective memory management will ensure the computer is running to its full capability while decreasing run times. The user interface handles complex characterization for model setup and meshing. The updated interface handles these complexities, is easier to use, and ensures correct usage.

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Category: Computing
Type: Individual Poster Presentation
LA-UR: 14-25473

Challenges of Code Optimization and Compatibility When Cross Compiling

Cross compilation poses a number of different obstacles including change of processor architecture, differences in the operating system, and other incompatibilities that are inherent to the program. The LaGriT mesh generation toolbox developed at Los Alamos National Laboratories offered each of these obstacles in the process of its Windows cross compilation. This paper discusses the methods used to overcome these challenges in order to release the final cross compiled product.

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Type: Group Poster Presentation
LA-UR: 14-25524

Particle Methods for Future Architectures

As the scale of physical simulations moves to exascale and beyond, the use of highly parallel algorithms is becoming increasingly important. Future hardware appears to be following a trend where improvements in the clock, memory transfer and DRAM latency rates have stagnated relative to the overall number of computational cores available. If parallelized with care, many particle methods fit naturally into this ‘new^1’ approach at scientific computation.

Libparty is a library for large-scale particle simulations targeted specifically at this highly parallel model of computation. This library implements a number of common algorithms and data structures relevant to parallel particle simulation. Currently, the library’s methods are being targeted to scale well with a large number of Intel’s Phi coprocessors and Knight’s Landing processors.

In this poster, we address the parallel performance benefits of various data structures available in libparty. The data structures were tested for scaling with respect to the number of threads and the number of particles.

Name: Meghan McDonald
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Group: ISR-3
Mentor: Steven Brumby
Category: Computing
Type: Individual Poster Presentation
LA-UR: 14-25586

Categorization of Social Media Videos Using Deep-Learning Algorithm

Deep learning has been successful for categorizing still images, but has yet to be applied to social media video. In order to categorize videos we applied UC Berkeley and Google's open source Caffe algorithm to Twitter Vine 6-second public social media videos that we labeled by hand into separate categories. We then used our manually labeled set of approximately 1,500 Twitter Vine videos to calculate the accuracy and speed of processing of the Caffe algorithm. The objective was for the algorithm to recognize the objects in the videos without depending on the text. We compare results to both the Tweet text and of the human labeling of the visual content.

Name: Austin Orr
Program: UGS
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Group: DCS-CSD
Mentor: Rosie Romero
Category: Computing
Type: Individual Poster Presentation
LA-UR: 14-25414

ESD QC Testing Process

At the Los Alamos National Laboratory, a great deal of work gets put into ensuring that the software used by researchers, scientists, and other employees is safe to use and meets standards set by Los Alamos National Laboratory. As a result, the DCS-CSD QC testing team was formed in order to meet those standards. Through both the ESD (Electronic Software Distribution) website and the ESDZone application, the user can obtain software that he/she owns a license for. In order to simulate an employee attempting to install software using these methods, the QC testing process starts on the ESD webpage for the software being tested. The tester first reviews the information surrounding the application being tested to ensure correctness and applicability in order to avoid future confusion. After the information is reviewed, the tester begins testing the software itself using different scenarios. The tester will use multiple machines, physical or virtual, to test scenarios where the application being tested is either upgraded from a previous version (upgrade scenario) or installed on a machine with no previous version installed (new install scenario). During the test, the tester will test the functionality of the software as well as confirm that the software meets the standards at the Los Alamos National Laboratory. Testing functionality means ensuring that the application executes correctly and does not lose any functions at any point in the process. Testing standards mean confirming that the software does not try to make an external connection that cannot be disabled. Once the software goes through the testing process and passes all of the tests, it is released to other ESD technicians to be distributed throughout the Los Alamos National Laboratory.

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Name: Andre Grosset
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Name: Erin Carrier
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School: University of Illinois Urbana-Champaign

Name: Robert Pavel
Program: GRA
School: University of Delaware

Name: Andrew Reisner
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Name: Kenneth Czuprynski
Program: GRA
School: University of Iowa

Group(s): CCS-7
Mentors: Benjamin Bergen and Allen McPherson
Category: Computing
Type: Group Poster Presentation
LA-UR: 14-25562

Co-Design Summer School 2014

Hydrodynamics simulations with shock discontinuities arise in a variety of application domains. Due to the large size of many application problems, it is not feasible to solve the entire problem on a uniform grid, as the resulting simulations are both computationally expensive and memory intensive. To combat this issue, adaptive mesh refinement (AMR) is often used in order to limit both computational cost and memory use while achieving the desired accuracy. This project implements hydrodynamics simulations based on the Euler equations using a second order Finite Volume Method with AMR.

Additionally, a growing trend in the field of scientific computing is the utilization of system-level runtimes to provide a more intuitive means of exploiting the available parallelism of an algorithm. These tools are also able to simplify some of the challenges presented by data placement and load balancing. To this end, we have performed a survey of contemporary runtime systems with a focus on the inherent challenges of adaptive mesh refinement and have implemented our application in Charm++, HPX, and Intel's Concurrent Collections.

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Category: Computing
Type: Group Poster Presentation
LA-UR: 14-25649

A Low-Cost Technique for Power Measurement of Computer Components

In recent years, power consumption in large computing platforms has become a great concern for research facilities requiring high performance computing. To address this growing concern, computer scientists and engineers have explored numerous solutions to optimize system performance while reducing overall energy requirements. The Department of Energy has been focusing on specific methodologies that would aid in lowering the overall energy footprint of these large platforms. One such focus is determining how varying programming approaches compare in terms of both performance and overall system power consumption. Power models developed by the department require accurate verification through simple high-speed, high-resolution power monitoring techniques. Microcontrollers were assessed as one such viable option that meet those performance criteria. The utilization of these boards combined with an array of shunt resistors and instrumentation amplifiers provides a low cost avenue for tracking power expenditure amongst individual components in a small computing platform. Data records from the sensors were collected and stored during specific runtime operations of scientific applications.

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Group: DCS-CSD
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Category: Computing
Type: Individual Poster Presentation
LA-UR: 14-25467

Linux Unified Key Setup (LUKS)

There are Linux users looking for PTR's that currently are required to use self-encrypting drives (SED's), LUKS is an alternative software based encryption. The purpose of LUKS is to provide a unified key encryption with security access for administrators as well as a satellite server oversight for verification of the encryption. This encryption also needs to have shared password access. A clear testing plan was created with testing documentation for each test. The test will be performed on all standard machines that could potentially require this encryption. As testing progresses LUKS appears to be a viable solution for the requirements. Further with testing the encryption process is being clearly defined for the encryption technicians and field techs. More testing will verify this is a solution for all machines.

Name: Cameron Tauxe
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Group: EES-16
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Category: Computing
Type: Individual Poster Presentation
LA-UR: 14-25966

Introducing jFehm: A new, easier way to create FEHM simulations

While working with pyFehm (a Python interface for using FEHM), I found it confusing and frustrating to create simulations. Sure, the Python modules made the process easier than writing input files by hand, but I still felt like more improvements could be made. So I set to work creating a new program in Java to simplify the process even more. This program uses a graphical interface to create simple simulations. Someone can use to create a whole simulation without even seeing (let alone, writing) a single line of code. My poster showcases many of the features and the usability of this program.

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Group: XCP-4
Mentor: Nathaniel Morgan
Category: Computing
Type: Individual Poster Presentation
LA-UR: 14-25688

3D Lagrange Hydro

The Project consisted of testing a new algorithm inside of the FLAG (Free LAGrangian) program utilized by LANL Los Alamos National Laboratory (LANL).
The method is a 3D Lagrangian staggered grid hydrodynamic (SGH) Godunov-like approach that uses a Multi-directional Approximate Riemann Solution (MARS) method developed by Morgan et al. (2014). The objective of the summer research was to quantify the accuracy of the algorithm based on test cases with known analytic solutions that the numeric results can be compared to.

Name: Joseph Bakarji
Program: GRA
School: University of California San Diego
Group: EES-16
Mentor: Velimir Vesselinov
Category: Earth and Space Science
Type: Individual Poster Presentation
LA-UR: 14-25669

A Social Dynamics Dependent Water Supply Well Contamination Model

Contaminant concentration in water supply wells located near contaminant plumes depends on the pumping rate at those wells. In addition, the pumping rate depends on the amount of water used by the society. We simulate a scenario with (1) a physics-based model predicting contaminant-concentration at the water-supply well and (2) a social model based upon the consistency-conformity model to predict the water-supply needs. Accordingly, a water-supply well contamination model is coupled with different social dynamics models to predict the conformity rate of society as a function of the contamination concentration in water supply and the frequency of informative events presented to the public.

Name: Eric Benner
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School: University of New Mexico
Group: EES-16
Mentor: Velimir Vesselinov
Category: Earth and Space Science
Type: Individual Poster Presentation
LA-UR: 14-25668

Residual Analysis of Well Pressure Data for Interpretation of Aquifer Tests

High-accuracy water level data are needed to determine the spatially and temporarily variable hydraulic response to pumping in aquifers. However, the water-level data are typically affected by physical process unrelated to the aquifer pumping such as barometric pressure changes, tides, earthquakes, etc. We correct for barometric and Earth tide effects using linear regression deconvolution, as an initial guess for a nonlinear residual minimization to account for pumping effects. The pumping effects are incorporated using the Theis equation. In the future we plan to adapt the data for jumps due to recalibration. After minimizing the noise in this way, the data can be used to determine the storativity and transmissivity of the aquifer from the pumping data. The analyses also provide information about the accuracy of the collected water-level data.

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Group: ENV-CP
Mentor: Jean Dewart
Category: Earth and Space Science
Type: Individual Poster Presentation
LA-UR: 14-25500

Dose Assessment of Diffuse Sources for Los Alamos National Laboratory

The regulatory limits established by the EPA through the National Emission Standards for Hazardous Air Pollutants for Emissions of Radionuclides Other than Radon (Rad-NESHAP) authorizes a 10-millirem annual dose equivalent concentration limit from airborne emissions of radionuclides at LANL. The radiological air sampling network (AIRNET) measures concentrations of airborne environmental radionuclides in regions that the members of the public are located beyond LANL boundaries. An annual average dose and risk was calculated using a Gaussian plume atmospheric dispersion model in each of the 16 compass directions from radionuclide emissions by non-point (diffuse) sources, to assure that an AIRNET station is located in every downwind direction where the public is located. In order to ensure a high probability of AIRNET detecting a 2-hour or 8-hour release, a potential plume width was estimated from on-site measurements of the wind direction and standard deviation of wind direction ($\sigma\theta$). The annual average wind direction is predominantly a westerly direction at night and changes to a south-southwesterly direction throughout the day, and $\sigma\theta$ ranges from 13° at night to a maximum of 29° during the day. For a receptor located 1 km away from an emission source with a $\sigma\theta$ value of 13°, the monitors must be separated by 230 m in order to measure the release. While more downwind monitors would be required for such a release, a $2\sigma\theta$ value is used to estimate 95% of the plume resulting in an angle larger than one sector, 22.5°.

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Type: Individual Poster Presentation
LA-UR: 14-25485

Can We See Climate Change in LANL Meteorology Data? A Preliminary Review

One of the primary predictions of the Intergovernmental Panel on Climate Change (IPCC) for the Southwest United States is warmer temperatures and more intense short-term rainfall events. We will take a preliminary look at the temperature and precipitation data from LANL to determine if these impacts are present. We have already witnessed that the past decade has been the hottest on record, but are seeking to discover if the past 30 years show any trends. Owing to these temperature increases, there have been more frequent and widespread forest fires. This may also lead to water shortages, the core concern for the desert southwest. Here at LANL, we have five weather towers spread out across the property. These towers measure wind variables, atmospheric state variables, precipitation variables, and radiative fluxes. This project will focus on trends of temperature and precipitation over the past 30 years and in the most recent decade. We will also examine the frequency and number of occurrences of heavy precipitation during a short time interval, and how these patterns have evolved over time.

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LA-UR: 14-25667

An Analysis of Recent Cases of Induced Seismicity in Arkansas and Oklahoma

Earthquakes are common in the western United States. More recently, the number of earthquakes in the central and eastern United States has been increasing; nearly doubling since the 1970s. It is likely that the increased seismicity can be attributed to wastewater injection from Oil and Gas operations. Induced seismicity is the triggering of earthquake activity by anthropogenic causes, which ultimately leads to the release of energy on the Earth's crust. Earthquakes can be triggered by mining operations, reservoir impoundment and fluid injection, all of which affect the pore pressure and subsurface stress state that control the mechanisms for induced seismicity. According to Horton [2012, the U.S Environmental Protection Agency provides injection control regulations to protect underground sources of drinking water; however, it does not limit the proximity of waste disposal wells to active seismic zones, hospitals, nuclear power plants or other important facilities.

The aim of my research project is to develop a database of known sequences of induced seismicity to complement recent modeling efforts at LANL. This involves finding and processing induced earthquake catalogues as well as the injection conditions presumed to have caused these events. So far I have documented two induced earthquake sequences: Guy, Arkansas in 2010-11, and Prague, Oklahoma, in 2011-12. One of the differences between these sequences is that injection operated for 17 years in Oklahoma before a significant increase in the rate of seismicity was observed. I have developed an Excel spreadsheet tool to so that the induced seismicity databases can be filtered by magnitude, timing and location and visualized against the injection data or on a map. Conducting research on these earthquake sequences contributes to a longer term goal of being able to forecast the risk of induced seismicity.

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LA-UR: 14-25458

Visualizing Chromium Concentrations near the Los Alamos Water Table

Chromium used as a corrosion inhibitor in a LANL power plant was historically released as effluent into the headwaters of Sandia Canyon. Several wells are being used to monitor the concentrations of chromium in perched intermediate and regional groundwater. Although chromium is found beneath the water table, chromium has not been detected in deeper regional water supply wells. The measurements from these wells, while useful snapshots in time and space, are not, by themselves, effective in determining how the subsurface chromium plume is moving. In order to help remedy this, a model was created to interpolate the full plume and display its changes and movement over time. This is the Chromium Visualization Tool. Written in Java using JavaFX, the Chromium Visualization Tool shows the concentration at each well location over time. The ability to interpolate between well locations to create a 2D plume at each timestep is currently being added. The end goal is to display a plume for each of several depth ranges at every timestep to provide an accurate visualization of how the chromium is being transported in the subsurface and to facilitate predictions of future movement.

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Monitoring the Stability and Biogeochemistry of the Sandia Canyon Wetland

The Sandia Canyon Wetland is an effluent supported wetland sustained by three National Pollutant Discharge Elimination System (NPDES) permitted outfalls. The volume of water discharged into the wetland has decreased since July 2012 when the Sanitary Effluent Reclamation Facility (SERF) began full scale operation. SERF provides tertiary treatment to treated water from the Sanitary Waste Water System (SWWS). SERF was constructed to meet more stringent water quality regulations as well as to reduce the Laboratory's consumption of potable water in surrounding cooling towers. SERF has resulted in a reduction of the volume and a change in the chemistry of the water discharged into the wetland. A grade control structure was installed at the terminus of the wetland to reduce erosion, to help maintain saturation, and to promote reducing conditions within the wetland. Stabilizing and maintaining reducing conditions within the wetland will help prevent mobilization of contaminants present in the wetland sediments. A network of 13 alluvial piezometers was installed throughout the wetland to monitor the hydrology and biogeochemistry of the groundwater resulting from SERF operation and the installation of the grade control structure. The piezometer water level data indicates that the wetland has remained saturated while the low nitrate and sulfate concentrations in addition to the presence of ammonia and sulfide within the wetland suggest that reducing conditions are being maintained. Over the period of surveillance for this project, adverse effects were not observed within the wetland due to the reduction of water volume or changes in water chemistry of the incoming water.

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Hydrologic Impacts of Burn Severity on Nutrient Concentrations

Climate change is currently intensifying wildfire behavior and thus fire severity in the Southwest. Following large fires, or “mega-fires,” surface water runoff contributes high concentrations of nutrients to water bodies, which has the potential to impair surface water quality in the receiving aquatic systems. The purpose of this study was to investigate the contributions of total suspended solids (TSS), nitrate-nitrogen (NO3-N) and orthophosphate (PO4) concentrations in surface water runoff originating from high, moderate, low, mixed, and control (unburned site) fire severity types from the Las Conchas fire in the Jemez Mountains, New Mexico. ISCO automated water samplers and buried single stage water-samplers were used to collect surface water runoff from ten precipitation events during the 2012 monsoon season. Total suspended solids was measured from surface runoff was collected from amixed severity site as well. TSS, NO3-N, and PO4 concentrations were determined following standard Environmental Protection Agency (EPA) methodology. TSS was determined using a gravimetric method and nitrogen and phosphate t concentrations were determined using colorimetric methods using an OI Analytical Auto Analyzer. Preliminary results show that TSS were highest from the mixed severity site and increased with fire severity from Low to Moderate, to High severity burn. Additionally, NO3-N concentrations in surface runoff also increased with fire severity. TSS concentrations ranged from 3 mg/L to 28 mg/L; NO3 concentrations ranged from 3.1 mg/L at the Control site to 7.8 mg/L at the High severity site. PO4 concentrations decreased with fire severity, ranging from 0.35 mg/L at the Control site to 0.1 mg/L at the High severity site. Data from all burned severity classes were collapsed, or merged, resulting in the average NO3-N, and PO4 nutrient concentrations between burned and unburned (Control) sites being significantly different ($p<.001$). Results from the Las Conchas fire illustrate the potential for nutrient loading in runoff that may result from high severity wildfires. Our findings suggest that large wildfires or “mega-fires” experience amplified nutrient modifications and can pose negative water quality effects on receiving aquatic systems.

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LA-UR: 14-25569

An Analysis of Resin Flow in Pinus Edulis Due to Fungal Inoculation

Intense bouts of heat and drought due to climate change carry more consequences for piñon pine (Pinus edulis) than meets the eye. The physiological stress put on piñon pine due to heat and drought in the Southwest United States can lead to greater vulnerability to pathogenic attack, particularly by bark beetles (Ips confusus). Bark beetles bore into tree bark, lay eggs, and feed inside the bark of the tree. The Ips confusus bark beetle is associated with two types of fungi that can be detrimental to piñon pine: Ophiostoma sp. and Grosmannia clavigera. Piñon pine trees have two responses to bark beetle invasions, constitutive and induced. A constitutive response is one in which the tree releases a certain amount of resin already stored in the tree. An induced response is one in which the tree produces more resin in response to the bark beetle infestation. This experiment tested whether Pinus edulis displayed a constitutive or induced response when inoculated with cultured fungus, Ophiostoma sp. and Grosmannia clavigera. Fourteen experimental piñon pines underwent mechanical wounding and 7 were later exposed to the two bark beetle-associated fungi. We used metal funnels and 15-mL collection tubes to collect resin from the mechanical wound sites after 24 hours, 48 hours, and 7 days. We found no evidence of induced resin flow in Pinus edulis; instead results indicate this species utilizes a constitutive resin defense response. This finding indicates that during drought Pinus edulis trees must defend themselves with resin defenses acquired prior to bark beetle attack, with implications for predicting causes of tree mortality in this species.

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Inscribed Places: Examining Rock Art Landscapes on the Pajarito Plateau

At LANL, one constantly encounters cultural materials of the past, whether it is the remains of research buildings utilized during the Manhattan Era, or the remnants of dwellings of Pre-Columbian farmers on the Pajarito Plateau. Rock art sites are often encountered places where images of various meanings have been physically pecked and scratched out by people inscribing their identities and their worldviews onto the surrounding landscape. Because a landscape can persist in form and memory in various states of visitation, deterioration, and commemoration, we need to view rock art in relation to surrounding habitation and cultural activity sites, as well as natural resources at various scales. I take a landscape approach combining Puebloan ethnography and GIS applications to examine approximately 150 rock art sites in the LANL cultural resources database dating from A.D. 600 - 1600. This approach allows for robust recognition of spatial and temporal patterns, such as the range of variation in terms of topographic settings through time. Are there differences in where certain motifs can be seen and accessed, and conversely, are there places where certain images are not depicted and cannot be viewed? Can we identify differences between interior cavate or kiva art and isolated petroglyph panels? My initial results suggest there are spatial patterns among rock art motifs and their placements on cliff faces along the cardinal directions, specifically North and South. My findings indicate that this pattern persists over a long period of time and is related to a common ideological practice. By examining these questions and using a landscape approach, my research contributes to a wider social understanding of the significance of these inscribed places to peoples of the past, present and future. It also informs how we can experience these places on LANL property and what we take away from them.

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LA-UR: 14-25811

Urban Storm Water Runoff

Under the national pollutant discharge elimination system (NPDES) Individual Permit, Los Alamos National Laboratories monitors stormwater discharge from solid waste management units (SWMUs). Stormwater 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, stormwater 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 stormwater 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 stormwater running-on to SMAs adjacent to urban and industrial environments and compare those results with what is flowing off of the SMAs. Global Water automated sampler's were deployed and are currently maintained on a regular basis throughout the monitoring season and stormwater 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 stormwater runoff.

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Comparing Wildlife Activity in Two Wetlands Using Motion Triggered Cameras

In Northern New Mexico, wetlands support a unique and varied ecosystem as well as providing wildlife with valuable sources of water. Within Los Alamos National Laboratory (LANL) property, there are two main wetlands; the Sandia and Pajarito Wetlands. The Sandia Wetlands is fed primarily by an outfall from Technical Area 3, but also from storm water runoff from multiple parking lots that are above the wetlands. The Pajarito Wetlands, however, is fed entirely from natural sources and is not close to any technical areas or parking lots; thus making it more susceptible to drought conditions. As LANL shares its property with a plethora of wildlife, it is important to understand how the work being done affects the environment and therefore how best to manage the land. Factors that may affect the wetlands and the wildlife that use them include amount of water, vegetation type, development, and human interactions. In order to monitor and compare the species and their frequencies, three remote cameras were deployed at each wetland in January 2014 and were checked monthly for positive images. These images were then analyzed for species, number of individuals, sex, and whether there were young present. After six months of the study, the results show that although both wetlands had many animals, the animals which were most frequent varied at each site. Most of the images captured at Sandia Wetlands were of deer, whereas at Pajarito Wetlands elk were the most prevalent. The sites captured different predators as well; with a bobcat and a mountain lion being seen at Pajarito Wetlands, and a black bear at Sandia Wetlands. Other common animals captured were coyote, rabbit, and squirrel. Studies like these can help LANL make more informed management decisions for the benefit of both the employees and wildlife.

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LA-UR: 14-25591

Ecosystem Health Evaluation: Environmental and Anthropogenic Impacts on Birds

The Avian Nestbox Network (ANN) was started in 1997 by Dr. Jeanne Fair. Hundreds of nestboxes were placed in nesting habitat throughout the canyons and mesa tops surrounding LANL facilities. The purpose of the ANN is to monitor and evaluate the effects of naturally occurring and anthropogenic factors on the health and productivity of bird populations on and around LANL property. Long-term studies like this contribute to a better understanding of bird populations and ecosystem health. The Western Bluebird (Sialia mexicana) and the Ash-throated Flycatcher (Myiarchus cinerascens) are the two species of focus. They are cavity-nesting species with similar life histories and habitat requirements, but are significantly different in size and nestling growth rates. Important population parameters that have been studied using the ANN include: feeding habits, reproductive success, nestling sex ratios, immunological changes, physical changes in eggs, and parasite loads. In 2014, we checked the nestboxes every two weeks throughout the breeding season to find active nests. Active nests were closely monitored until the nestlings were old enough to band and sex. The location of the box, species, band number, and sex were all recorded for each nestling. We compared active nests from 2014 with previous years to test whether birds' preferences for nesting locations has changed over time. Temperature data loggers were added to the nestbox network in 2014 to monitor internal and ambient temperatures of the nestboxes. Temperature is a very important aspect for bird nesting success, and is important for understanding changes in bird nesting behavior and the potential long term ecological effects as climate continues to change. Our nesting data indicates that the target species are now nesting in higher elevations. Preliminary indications from the temperature data suggest that lower temperatures could attribute more to nest failures than higher temperatures.

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LA-UR: 14-25666

Modeling and Simulation of Induced Seismicity Using the Rate-State Method

Earthquakes are the result of a sudden release of energy from the Earth's crust that creates seismic waves. Earthquakes are a natural occurrence; however, due to injection of fluid into the ground, they are becoming more frequent in regions of historically low seismicity, e.g., the central and eastern United States. Injection-induced earthquakes are caused by injected wastewater, or other fluid, e.g., CO2, that create pressure change below the surface, which the initiate seismic activity. A July 2013 study by US Geological Survey scientists has shown the dramatic effects of injection of wastewater on induced seismicity. Over a three year period, the number of earthquakes of magnitude 3.0 or greater in the central and eastern United States increased dramatically from 21 events/year to as high as 188 event/year. At some of the locations there was a direct relationship between injection and seismic activity. Injecting fluid into the ground raises subsurface pressure and causes stress and friction to become unbalanced; this can lead to an earthquake. We have modeled this process using the earthquake simulator PyLith. PyLith is a modeling application used to simulate earthquakes and examine the displacement and stress changes. The work-flow structure consists of creating the geological structure; mesh generation, implementing the relevant physics, and visualization of results. Applying a rate-and-state method for fault friction, as well as point forces and fault tractions to represent the fluid intrusion, we approximated an induced earthquake resulting from fluid injection in Oklahoma in 2011. Recreating this scenario has given us the ability to examine more closely what forces are affecting the seismicity and is a step toward methods for forecasting induced seismicity.

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A Column Analog Study of the Natural Attenuation of U at an ISR Mining Site

Since the 1960's, in-situ leaching technology has been utilized to mine uranium (U) from low-grade roll-front ore deposits. An injected lixiviant solution oxidizes most U(IV) to U(VI) and dissolves the U(VI) as aqueous complexes, thereby mobilizing U into the groundwater for subsequent recovery. When mining is complete, the subsurface chemistry is significantly altered, and residual U concentrations in the ore zone water are typically much higher than before mining, which poses environmental concerns. The goal of this study is to examine the mechanism and extent of the natural attenuation of U provided by local sediments downgradient of a mining zone at Cameco Resources' Smith Ranch Mine (Wyoming). Three mineralogically distinct sections were sampled from a core collected downgradient of the ore zone in an unmined sandstone unit and packed into three separate columns (A, B, and C). Visual inspection indicated more organic content present in the material in Columns A and B than in Column C. Ore zone groundwater from a mined unit, containing high U concentrations, was flowed through the columns under anaerobic field conditions over several weeks. The groundwater was spiked with tritium, a conservative tracer, and filtered to limit microbial activity. Comparisons of the tritium and U breakthrough curves show recoveries of 87% and 98% of the total U injected in Columns B and C, respectively (Column A results are pending after two planned flow interruptions). The greater retention of U in Column B could be due to reduction of U(VI) to U(IV) by pyrite (FeS) or carbonaceous matter and subsequent deposition in this reducing environment. Future comparisons of U distribution and speciation in unreacted and reacted column sediments by optical microscopy, X-ray Fluorescence, and X-ray Absorption Fine Structure spectroscopy should provide insights into the natural attenuation processes occurring in the columns.

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LA-UR: 14-25703

Development and Qualification of Optical Profilometer for Detonator Inspection

The current process for Inspection of detonator cup scratches, pits and dents is done through defect reference standards and the use of the light section microscope. The light section microscope uses a fine band of light to trace a profile of the peaks and valleys of a surface; an operator moves the micrometer reticle from the peak to the valley of the band to obtain the depth of the scratch pit or dent. This requires an operator with large amount of skill and practice with the machine to maintain its accuracy of ±1µm. On average the light section microscope take 5 to 15 minutes to evaluate the depth of an imperfection.

Optical profilometry uses nondestructive measurement using interferometry to construct a three dimensional surface profile of the part, scratch, pit or dent. This is done by splitting the light within the objective; one portion reflects from the test surface and another portion reflects from a reference surface within the objective. Interference between the two light wavefronts creates "fringes" that the solid-state camera and software can convert into height maps to construct a surface profile. Using the optical profilometer removes the subjectivity between inspectors.

Using optical profilometry, an operator with minimal skill is able to evaluate an imperfection with twice the accuracy and at least a 66% improvement in efficiency. To certify the system for production use, the machine had to be qualified to measure the depth of scratches, pits and dents with a Test Uncertainty Ratio of 4 to 1. This was done by running a gage reproducibility and repeatability with 10 pre-scratched cup and three different inspectors. To develop process specific programs, fixtures were designed and built to help improve ease of use as and decrease variability in-between measurements.

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Type: Group Poster Presentation
LA-UR: 14-25360

Mobile Robotic Automation of Nuclear Material Operations at TA-55

In order to increase safety and reduce the radiation dosage to personnel in mission-critical nuclear activities at the laboratory, new robotic systems must be developed to accomplish tasks currently performed by human workers. To this end, the laboratory is working in conjunction with the Nuclear Robotics Group at the University of Texas at Austin to design and deploy a mobile platform for service in the Plutonium Facility at TA-55.

The primary mission of the system is to manipulate and transport containers of hazardous nuclear material, including plutonium, to and from the PF-4 nuclear material vault. Additional planned capabilities include autonomous inventory of material, routine radiation and criticality surveying, and security monitoring. The vault contains very intense radiation fields, and personnel currently performing such work receive very high doses. Tasks must be performed quickly and personnel are rotated to avoid exceeding exposure limits. The use of robotic systems will greatly reduce the need for such onerous practices and allow radiation workers to spend their exposure allowances on other activities.

This poster presents the current state of development on the system. The current prototype features both autonomous and teleoperated behavior. Autonomy will be achieved using LIDAR vision, inertial sensors, and SLAM (Simultaneous Localization and Mapping) algorithms. Point cloud mapping will be used to identify changes in a scene (security anomalies such as containers missing, doors left open, etc) during morning room inspection. In addition, software has been developed to integrate radiation sensors and perform autonomous surveying and 3-D mapping of radiation fields, and to visually display data for the operator. Work has also been completed to improve the kinematic reliability and safety of manipulator arms while performing uncertain tasks.

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Category: Engineering
Type: Group Poster Presentation
LA-UR: 14-25954

Storm Water Control Structure Matrial Selection

Storm water control structures are used to restrict or contain surface runoff that may contain elevated levels of contaminants. The goal of this study is to establish a cost basis for the design of storm water control structures at typical locations at Los Alamos National Laboratory. Locations were selected based on size and type of structure, which is dependent on the watershed and site specific characteristics. The viability of precast concrete, cast-in-place concrete, gabion baskets and earthen berms are evaluated with respect to performance requirements and environmental conditions at each site. The evaluation criterion includes retention/detention capacity, impact resistance, land requirements, longevity, long term maintenance, watershed size, and design considerations.

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Type: Group Poster Presentation
LA-UR: 14-25785

Creating a Tool to Analyze CMM Data with MathCad

There are many different techniques used to determine if a part is useable according to the design requirements. One technique often used is a coordinate measuring machine (CMM), which provides a set of Cartesian coordinate data that corresponds to points on a part. CMM data can be evaluated to determine if the idiosyncrasies in shape are within a designer's tolerance. Not all measurements of interest can be verified using raw CMM data and the accompanying programs. One measurement of interest to designers for a spherical part is the radial wall thickness, which can greatly impact the structural integrity of a given part. The current process used to analyze the CMM data to determine the radial wall thickness is very labor intensive requiring the sequential use of Microsoft Excel and CREO Parametric, which have minimal compatibility. The objective for this project was to create a program that calculates the radial wall thickness from a set of CMM data, requiring little user input. MathCad Prime 3.0, a software intended to perform engineering calculations was chosen, due to its ease of use and its high compatibility with all PTC products including CREO Parametric. Using the Mathcad a tool was created that allows a user to input the CMM data and, with minimal user inputs, it will determine an approximation of the deviation from nominal radial wall thickness. The program formats the data for compatibility with CREO Parametric's 'Verify' feature, allowing the user to see a 3-dimensional view of the nominal object, as well as the real-world part's deviations from nominal. This program has the capability to reduce an hours long, labor intensive process into a program which takes less than 10 minutes to run and requires far less effort.

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Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25644

Thinking computational physics outside the PDE framework: The Cell Method

I will present the formulation, implementation, and application of a numerical technique for elastodynamics that is fast and geometrically flexible. The numerical technique is based on the Cell Method from Enzo Tonti, which uses elements of algebraic topology to formulate the physics in discrete form, without ever using the differential formulation and the limit process associated with it. I have worked on implementing this technique into a practical computer code written in MATLAB. The accuracy and speed of the code is verified against numerical solutions obtained with a commercial software package: COMSOL Multiphysics. After this verification, the code was applied in the context of non-destructive evaluation, to detect the presence of damage on the surface of a solid sample. The detection technique combines the principle of time reversal to the properties of nonlinear acoustics.

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Type: Group Poster Presentation
LA-UR: 14-25459

Technical Support for Irrigation Water Loss Effect on Agriculture

This study is aimed at establishing a more efficient water allocation system in the Arch Hurley Irrigation District to aid in economic distress plaguing the local community. Over the past 50 years, the Tucumcari, New Mexico area has seen a significant reduction in the District's surface water supply. This reduction can be attributed to chronic drought and high water loss sections of the open canal, due to evaporation and infiltration . Water shortages have led the District to conserve available water by allotting a "premium" rate per acre-foot of water delivery which most local subscribers cannot afford. Plans to install a pipeline along the main canal to improve distribution efficiency have been proposed, however due to a lack of funding, this option has not been implemented.

The ultimate goal of this study is to identify one or more options that can generate sufficient electric power to support pumping and siphons along the Conchas canal, while also exporting excess electricity to the grid for resale. The proposed electric alternative options include: low-head hydro, solar arrays, wind turbines, and gas turbines with 500 kW electric capacities. Revenue generated from one of these preferred alternatives could potentially support pipeline installation along the canal to help mitigate future costs. Once a preferred alternative is selected, a life-cycle cost (LCC) analysis will be performed to estimate cost-benefits of constructing selected pipeline sections along the open canal. An installation and construction plan for the preferred alternative will be devised to provide net income over several extended phases of pipeline operation.

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Type: Group Poster Presentation
LA-UR: 14-25906

DARHT Axis I Automated Diverter System

The Dual Axis Radiographic Hydrodynamic Test facility, or DARHT for short, is a key piece of the nation's Stockpile Stewardship Plan. One of the worlds most advanced weapons test facilities, the facility consists of two powerful accelerators, DARHT Axis I and DARHT Axis II, centered on a target at a 90° angle. Each accelerator electron beam is focused onto a metal target that converts the beam’s kinetic energy into x-rays. Multiple x-ray pulses produce multiple-view radiographic images of a full-scale nonnuclear weapon mockup as it implodes. The final result is freeze-frame radiographs. These radiographic images are used to evaluate nuclear weapons through nonnuclear hydrodynamic testing.

One of the key machine safety components of the Axis I accelerator is known as the diverter. The diverter is an oil insulated spark gap in parallel with the Blumlein that will hold off the Blumlein voltage for 5µs, preventing continued ringing voltage on the Blumlein. This spark gap must be set at a specific distance and is adjusted with the PPT voltage. Because of this the diverter must be adjusted frequently.

Currently the diverter is adjusted manually using a hand crank located in the Axis I accelerator hall. In order to reduce the possibility of operator error and to interlock the system, it has been desired for some time to automate this system. We have been working on creating an automated system based off of work from a previous attempt at automating the diverter 10 years ago. This requires re-machining several key components, updating outdated parts, and making adjustments to parts of the control system from the old design.

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LA-UR: 14-25504

Computational Analysis of Buoyancy Driven Rayleigh-Taylor Mixing

Volumetric Energy Deposition (VED) by microwaves is being utilized to explore buoyancy driven mixing of miscible fluids. To further understand this phenomenon, a code is being developed to simulate the experimental setup. The experimental setup consists of two fluids, a less dense, weakly polar fluid (toluene) that lies on top of a denser, polar fluid (tetrahydrofuran). The two fluids are exposed to microwaves that slowly begin to heat both fluids. Tetrahydrofuran has a higher polarity and consequently absorbs the heat emitted by the microwaves at a faster rate, and because of thermal expansion it becomes less dense than the fluid placed on top. Thereafter, the two fluids begin to experience Rayleigh-Taylor instabilities and buoyancy driven mixing occurs. A Fortran 2D Cartesian code that contains an explicit method for advection, and an implicit method for continuity and pressure is the basis for the code needed to simulate the experiment. The code has been modified to solve the temperature transport equation, and to contain the density change that takes place when the fluids are exposed to the microwaves. The microwave power absorbed by the THF was incorporated to the code by inputting a source term in the temperature transport equation. To acquire the source term, the general microwave power equation was utilized. The only variable in the source term was the electric field strength, while the dielectric constant, vacuum permittivity, and frequency values were assumed to be constant. Throughout the process, the post-processor Ensight was utilized to analyze the results and to verify that the code was working correctly. The code provided contours for the temperature change, volume fraction, and velocities. The contour of the Rayleigh-Taylor mixing VED conditions is demonstrated.

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Group: W6
Mentor: Nate Sanchez
Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25770

Chip Slapper Detonator Testing Under Extreme Conditions

In order to analyze the effects of the external conditions of extreme cold temperature and intense vibration on the Chip Slapper Detonator and its respective components in the detonation process, we have developed and conducted a series of tests at varying voltages designed to illustrate the shock wave propagation emitted over time from the slapper system. Both Hardfire and Neyer tests were conducted at conditions of extreme cold and a post vibration state in order that each condition was evaluated at a given voltage for the Hardfire testing, and evaluated again at varying voltages across the band of Neyer tests. Neyer testing is based off of the Barry T. Neyer program calculating the threshold voltage needed to initiate detonation in a given system. For these test series we chose to use a chip slapper detonator in conjunction with a PETN explosive pellet of 1.65 g/cm^3 compressed density, initiated by a LANL TSD fire set. Using a digital streak camera we were able to obtain high quality streak images of the detonation process and evaluate the precise timing of the breakout and center of initiation using a MATLAB Graphical User Interface (GUI) code developed by W-6. Once all individual condition tests are conducted we will then begin to evaluate timing of detonation across combinations of conditions in order to evaluate the detonators resilience to the combined environments of extreme cold and intense vibration.

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Group(s): WX-1
Mentor: Travis Weaver
Category: Engineering
Type: Group Poster Presentation
LA-UR: 14-25474

Do You Like it Hot or Cold?

The Dual Axis Radiographic Hydrodynamic Test (DARHT) Facility utilizes a cutting-edge accelerator design to provide radiographic images of hydrodynamic tests in order to provide valuable information for the Nuclear Weapons Stockpile Stewardship Program. As the stewardship program continues, enhanced radiography is needed and new designs will be employed so that the critical models of the program can be verified. There are currently two accelerator designs at the DARHT facility. These two differ from the very beginning and have much to do with a region referred to as the injector. Axis I accelerator uses a cold cathode made up of a velvet material to provide the electrons necessary for beam formation. Axis II uses a thermionic cathode that is made of metal and is heated to nominally 1100 °C for electron emission. In the Axis I injector, the system encompassing the cathode and anode regions, there are several components that are being analyzed for future accelerator designs. One of these components is a radial resistor, made of cross-linked polystyrene under the trademark Rexolite, which must be analyzed to determine the outgassing on the region under high vacuum and varying temperature. Besides Rexolite, there is also concern for the amount of other free molecules like water or silicates, which are known to have adverse effects on the injector region, specifically for thermionic cathodes. Using a Residual Gas Analyzer (RGA) to detect and quantify the amounts of released gas particles into the Axis I injector region, we will determine whether the Axis I design is favorable over the current Axis II injector design.

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Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-26134

Design, Fabrication and Testing of a Muffle Furnace Insulation Guard

Oxidation of actinide metals and stabilization of resultant oxides remains a focus of both Advanced Recovery Integrated Extraction System (ARIES) and Materials Recycle and Reuse (MR&R) programmatic activities. These processes are achieved through heating of actinide material in a radiological glovebox air atmosphere within a muffle furnace. Heating profile data is measured through several K-type thermocouples and is recorded for confirmation of material stabilization. Two of these thermocouples are placed within the bed of the actinide material. Placement of these thermocouples requires access holes through the top of the furnace body, through brittle vitreous aluminosilicate insulation, and into the actinide material bed. Processing has exposed two deficiencies related to placement and removal of thermocouples within the furnace. The first concerns contamination of stabilized material consistent with disturbance of friable furnace insulation. The second limitation is accurate placement of thermocouple within the material bed. A multi-functional muffle furnace thermocouple stay/insulation guard was designed, fabricated and tested. Details of the design process, fabrication and testing plan are presented.

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Group: NEN-5
Mentor: David Poston
Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25522

Nuclear Thermal Rocket Shielding

Traditional chemically-fueled rockets are inefficient for long-term, large payload space exploration missions. To achieve these desired long-term space missions the use of Nuclear Thermal Rockets are needed. The goal of this project is the design and optimization of the radiation shield for proposed Nuclear Thermal Rocket designs. The optimization parameters are the dose rate limits to electronics, equipment, and/or astronauts, as well as the overall weight of the system.

The approach taken here will be to model in MCNP6 the Nuclear Thermal Rocket, including lead gamma shield and lithium hydride neutron shield. Using MCNP6 the dose rate will be calculated for the region of interest. Multiple iterations of the shield design will be analyzed in attempts to best optimize dose rate and shield weight. Input or requirement on the two parameters may be provided from NASA in the future. The surface source write and surface source read functions of MCNP will be used for simplifying shield models and reduce computational time.

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Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25645

Evaluation and Cold Testing of Automated Material Reduction of Plutonium Pits

With a continually decaying surplus of nuclear weapons that are currently manually disassembled by glovebox workers, the University of Texas at Austin (UT Austin) has partnered with Los Alamos National Labs (LANL) to evaluate multiple proposed methods for automating plutonium pit reduction. Tools currently used to dismantle pits are clumsy, unwieldy, and potentially dangerous in the hands of human workers. Thus the objective is to automate the process to reduce or eliminate workplace injury, contamination, proliferation, and possibly loss of life. A carefully implemented glovebox automation procedure can provide a level of safety, reliability, and repeatability that pure human interaction cannot achieve.

Any method of automation must satisfy certain end goal constraints; each pit should be reduced to pieces that can fit into a LANL-defined crucible and all pit material should be accountable to within 0.5 grams. Additionally, the proposed process should strictly adhere to ALARA principles. The material reduction device is composed of two major components: a cutting mechanism and a feed mechanism. A micro-punch was chosen for this particular application due to its ability to reduce material into traceable slugs as opposed to random shavings and significantly lower vibration during operation. Materials for appropriate cold test surrogates were researched for future testing.

By utilizing ROS's (Robot Operating System) built-in collision detection system and accurate collision geometry, an industrial robot arm could be programmed to move (feed) a plutonium pit hemisphere in and out of the punch. The robot used this summer to prototype this task process was a 7-DOF (Degree of Freedom) Yaskawa Motoman industrial robot arm. Both a vacuum gripper and Robotiq 3-finger adaptive gripper were tested for the robot-pit surrogate interface. This process effectively negates the need for human interaction inside the glovebox for material reduction.

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Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25505

MCNP-TH: External Coupling of MCNP to a Multi-Channel Thermal-Hydraulic Solver

The Monte Carlo neutron transport code MCNP6 is widely used to estimate criticality, flux distributions, and fuel burnup of nuclear reactors. Its ability to model virtually any geometry and its use of continuous-energy cross sections allow it to achieve a very high degree of accuracy for a variety of reactor types, regardless of core geometry or neutron spectra.

Currently, MCNP cannot internally calculate material temperatures and densities for neutron transport. Thus, the user must estimate these quantities beforehand, typically providing average values over the volumes of interest. However, the density of materials present in the reactor directly impacts reaction rates through macroscopic cross sections, and the temperature affects the materials' microscopic cross section resonance structure via Doppler broadening. Thus, specifying accurate temperatures can have an important effect on flux distributions and fuel burnup.

A coupled thermal hydraulic-neutronics calculation can be achieved with either strong coupling, where the governing fluid flow and heat transport and neutron transport equations are solved simultaneously, or weak coupling with operator splitting. The MCNP-TH methodology uses external coupling, wherein the user provides an initial estimate of material temperatures and densities, an MCNP neutron transport solve is performed, the resulting power distribution is fed into the thermal-hydraulic code, and the resulting fuel and coolant temperatures and densities are then returned to MCNP and iteration occurs between the neutronic and thermal hydraulic calculations until the convergence criteria is satisfied. While not valid for transients and other types of safety analyses concerned with very small timescales, it is an acceptable method for depletion calculations and other investigations over long time scales. Linking a thermal hydraulic solver with MCNP provides a robust means for obtaining accurate material temperature and density information for the neutron transport solution, which will improve the accuracy of the flux distributions and burnup information estimated.

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Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25987

An Algorithm-Based Defect Analysis for Coordinate Measuring Machine Test Artifacts

In order to ensure the reliability of the enduring stockpile, accurate dimensional inspection of nuclear weapon components is of paramount importance. The existing convention for dimensional inspection of hemispherical shells employs custom-designed instruments to characterize critical component features. Although these instruments provide high data density measurements with acceptable measurement uncertainty they require a high degree of user expertise, are expensive to maintain and calibrate, and have excessive measurement times. These limitations have driven an initiative to adopt the use of commercially available coordinate measuring machines (CMM), which have achieved a level of measurement uncertainty commensurate with the requirements for dimensional inspection. The dimensional inspection of hemispherical shells with CMMs yields a point cloud of X, Y, and Z position data. For the purposes of manufacturing quality verification, it is favorable to fit point cloud data to the nominal part geometry, which is represented as a solid model, and calculate the deviations of the manufactured component from the nominal. This technique allows for visual inspection of part deviations but fails to provide a quantitative measure of the defect sources. A defect is a deviation in the inspection data that may be a manifestation of the measurement uncertainty, such as thermal error, or the part geometry, such as manufacturing defects. An algorithm to quantify these defects is being developed in addition to a platform for artificially inducing various geometric deviations into the inspection data as a means to test the defect analysis algorithm.

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Group: ISR-3
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Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-24615

Single Event Upset Detection and Correction in Virtex-5 FPGAs

Field programmable gate arrays (FPGAs) allow scientists and engineers to create complex digital designs via hardware description languages (HDLs). A static random access memory (SRAM) FPGA's function is determined by programming volatile configuration memory. FPGA configuration memory is subject to single event upsets (SEUs) in high radiation environments such as nuclear power plants, particle accelerators, and the space environment. An SEU occurs when an ion or proton strikes the sensitive region of a transistor and causes a bit in memory to change state. Digital designs in an FPGA may malfunction in the event of an SEU, which could lead to a system failure. To combat this problem an SEU detection and correction system for Virtex-5 FPGAs has been developed. Configuration memory frames are continuously read back, a cyclical redundancy check (CRC) value is computed, and is then compared to a known (precomputed) CRC value. In the event that the CRC values do not match, the FPGA is partially reconfigured with the correct configuration data. Simulating SEUs via frame corruption and partial reconfiguration has shown that SEUs may result in functional failure. Preliminary testing of the SEU detection/correction system has proven successful thus far by restoring the design under test to operational status after a failure has occurred. Radiation testing will be conducted in late August 2014 at the Lawrence Berkeley National Laboratory 88" cyclotron using 50 MeV protons. The test will provide assurance that the detection and correction of SEUs is functioning correctly. The system allows for FPGAs to be deployed in high radiation environments by maintaining system integrity.

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Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25499

Hardware and Image Processing for Improved Trajectory Estimation

The ultimate goal of this project is locating, tracking and predicting an object's path in three-dimensional space with minimal a priori knowledge. This would allow for a camera to track objects outside of its field of view, enabling a single camera to track multiple objects. Theoretical algorithms developed last year by Matchen and Nadler use an estimated parameter to eliminate the a priori requirement and minimize the least-squares error of a Taylor approximation to determine the trajectory and recover the location at any time. This part of the project is focused on verifying those algorithms by implementing the hardware and software necessary. Namely, a GoPro Hero 3 camera and accompanying gimbal are used to capture video footage. The footage is then sent to the computer, which uses algorithms in MATLAB to detect an object and track it throughout the frames. Continuing work will involve generating data such as camera rotation angle and speed to feed into the algorithms developed last year.

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Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25776

Photon Doppler Velocimetry (PDV) System

We built a new PDV system to add four more channels of data for our gas gun experiments at TA40 Chamber 9. The Photonic Doppler Velocimetry (PDV) was created in the early 2000's to replace the Velocity Interferometer System for Any Reflector (VISAR), a fairly expensive and difficult system to set-up. The PDV uses fiber optic components (instead of open laser beams, lenses and mirrors) to send and receive light to and from a moving target. The reflected light is Doppler-shifted, recombined with some un-shifted light and sent to a detector. The mixing of the Doppler shifted and un-shifted light creates a signal containing the beat frequency that is then recorded on a digitizer. PDV is easier to field than VISAR. One reason for this is that PDV uses fiber optics instead of an open beam. The data obtained from the PDV is also easily analyzed using Fast-Fourier transform techniques. The PDV can be applied to high explosive testing, including gas gun experiments. It can be used to determine the projectile velocity, impact time, and the tilt of the target or impactor.

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Group: W-14
Mentor: Brian Olsen
Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25827

Extending the Life of a Wobble Vacuum Pump

A wobble pump is currently used to establish a vacuum during experiments. In this project the original pump was redesigned to extend its service life and improve its performance. The unique rotating motion of the wobble pump head means that a compliant Teflon ring must be used to maintain a seal between the piston and the cylinder wall. When the pump is in storage for long periods, the current ring experiences creep and stops being able to provide an adequate seal. A kinematic linkage was designed that allows the Teflon ring to be stored outside of the piston cylinder when not in use. When the pump is turned on, the ring and piston head automatically enter the cylinder and operate normally. Design changes were also made to the pump to maximize the compression ratio. This allows the pump to reach a lower vacuum pressure than the prior design. A functional prototype of the design was produced.

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Group: NEN-5
Mentor: Michael Fensin
Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25638

Validating the Depletion Capability of MCNP6 and MONTEBURNS

The concentration of isotopes calculated by simulating different reactors to End-Of-Life using MCNP6 and MONTEBURNS was compared to the OECD/NEA's spent fuel composition database. A sensitivity analysis was conducted on different simulation parameters to determine how these parameters affect the error in the simulation. Due to lack of available full core model descriptions, we modeled a single assembly (with specular reflected boundaries) of a PWR, a AGR, and a CANDU. We used only one common temperature per material, and about 20 time steps for each of the simulations. The relative errors in the concentration of most of the isotopes at End-Of-Life were under 10% when compared to the OECD/NEA's spent fuel composition database.

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Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-26109

Measurement and Simulation of Cosmic Ray Effects on Neutron Multiplicity Counting

Neutron coincidence and multiplicity counting is a standard technique used to measure uranium and plutonium masses in unknown samples for nuclear safeguards. Time correlated neutron detectors and knowledge of fission neutron production are used to find the composition of the sample. Background sources of radiation can obscure the detector results resulting in higher minimum detectable sample mass. Uranium 238's low spontaneous fission production (1.3e-2 n/s/g) means that sample masses are frequently below the minimum detectable activity.

High energy cosmic rays can produce events with large neutron multiplicities, which give rise to large coincidence count contributions. Since some of the events occur in the sample itself, it is impossible to measure the background separately. For example, adding 22kg of lead to an empty chamber increased the doubles rate by a factor of 15. This effect greatly increases the limit of detection of some low level neutron coincidence counting applications. The newly-developed cosmic ray capability of MCNP6 was used to calculate the expected coincidence rates from cosmic rays for different sample configurations and experimental measurements were made for comparison. The results show that the new capability is adequate to predict the expected background rates.

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Group: W-6
Mentor: Steven Clarke
Category: Engineering
Type: Individual Poster Presentation
LA-UR: 14-25921

3-D Analysis of Explosive Performance Testing

Onion skin test have historically been one dimensional tests; providing good data along a 1-D, but basically wasting the rest of the detonator. For this reason, multidimensional tests are more desirable and the Furball (hemispherical) and Ding-Dong (cylindrical) tests are what have been designed for that the purpose. These tests produce 6 axis of data from which a more complete image of the detonators overall behavior. This requires the development of new analysis tools to allow for visualization of the 3-D data. "Furball_Analysis_GUI" was created for that specific purpose.

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Group: OSH-OM
Mentor: Cindy Lawton
Category: Health & Safety
Type: Individual Poster Presentation
LA-UR: 14-25772

Testing, Introduction, and Redesign of Glovebox Airlock Sliding Trays

Roughly 10,000 transfers through glovebox airlocks are performed during normal operations each year at LANL. These transfers involve a significant amount of shoulder rotation and are an integral cause of 28 recorded glovebox shoulder injuries. A magnetically mounted sliding tray was designed and manufactured to reduce the shoulder stress during airlock transfers, and will fit in the most common round airlocks in the Plutonium Facility (PF-4). However, PF-4's square airlocks and extra-long airlocks pose a very high risk of shoulder injury. Square airlocks are located in the machining area where workers tend to move heavier objects, and extra-long airlocks pose issues due to their length. Trays for the square airlocks were designed using 3D modeling software in order to prevent future injuries. Trays for the extra-long airlocks were designed to split into smaller sections because they would be too long for introduction via the overhead trolley system as a solid piece. These trays could then be assembled with relative ease inside the glovebox. To move forward with introduction, safe installation procedures were established through cold laboratory testing. A team consisting of glovebox workers, an ergonomist, and engineers developed a set of installation instructions for incorporation into an Integrated Work Document (IWD). Tray capabilities were also tested in the cold laboratory, including how magnet placement affects load-bearing ability, the tray length at which two magnets are required, and how the magnet interacts with the surrounding glovebox gauges. Additionally, it was determined that an improved method of transporting the trays in the trolley bucket was needed to improve safety. A wedge was designed to ensure safe transport to the designated airlock. Overall, the ergonomic improvement offered by the airlock sliding trays will help boost productivity, increase worker comfort, and most importantly reduce risk of injury.

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Group: RP-PROG
Mentor: Michelle Lee
Category: Health & Safety
Type: Individual Poster Presentation
LA-UR: 14-25624

The Comparison of Radiation Detection Methods Measuring Pulsed X-ray Beams

Los Alamos National Laboratory (LANL) is a multidisciplinary research institution dynamically engaged in technological innovations to impede nuclear threats and resolve issues concerned with the environment, public health, and global security. Whether deliberate or incidental, some work conducted at LANL encompasses the use of radiation generating devices (RGDs) (e.g., radiography, material analyses, security, emergency response, etc.). The RGD program at LANL ensures that regulatory requirements are implemented for RGD-related activities to keep worker exposures to radiological hazards as low as reasonably achievable (ALARA). The Radiation Protection Programs (RP-PROG) RGD Office uses various radiation detection methods to perform compliance surveys to characterize radiological hazards and recommend radiological controls and posting for RGD operations. Using data compiled from RGD compliance surveys, this study compares efficiencies of radiological detection methods by evaluating the primary beam radiation output of high energy pulsed Golden X-ray Sources.

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Category: Health & Safety
Type: Individual Poster Presentation
LA-UR: 14-25893

MCNP Modeling and Benchmarking of a Xenon Gas Proportional Counter

Exit monitors such as Hand and Foot Monitors and Personnel Contamination Monitors often alarm based on Radon daughter activity causing unnecessary delays and customer frustration. As a result, there is a need for an instrument that can quickly and accurately differentiate radon progeny from transuranic alpha activity on personnel and clothing. In this respect a xenon-based gas proportional probe coupled to a compact analyzer module has been evaluated as a potential solution. This instrument is capable of operating in a number of different measurement modes that could singly or in concert enable a rapid determination of the source term. The probe has also been modeled using MCNP and benchmarked against empirical data. It is hoped that the probe design can be optimized as a result of the MCNP calculations.

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Category: Health & Safety
Type: Individual Poster Presentation
LA-UR: 14-25892

An Approach to the Design of the LANL "NKOSOO" Alpha and Beta Sandwich Detector

A detector (LANL “Nkosoo" – Progress Sandwich) combining an alpha air proportional and beta plastic scintillator has been developed, with the aim of measuring alpha and beta surface contamination in the presence of gamma and neutron interference. The alpha and beta counting rate were indicated separately on PX and SX RadEye rate meters. It is shown that the new developed detector has 4π detection efficiencies of 25.7% and 22.0% for Pu-239 and Cl-36 respectively.

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Group: ENV-ES
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Category: Health & Safety
Type: Individual Poster Presentation
LA-UR: 14-25733

Radionuclides in Field Mice Upstream of the Los Alamos Canyon Retention Structure

Los Alamos Canyon contains radionuclides and chemicals from legacy releases at Los Alamos National Laboratory. Because of the Cerro Grande Fire, a flood retention structure (weir) was constructed across the channel in late 2000 to help contain sediments in the canyon from reaching the Rio Grande. Field mice are effective bio-monitors of environmental contamination and they were used to assess the transfer of LANL released substances to a mammalian receptor species. From 2007–2013 field mice (Peromyscus spp.) were collected each year under strict hanta virus protocols from behind the weir, and analyzed for plutonium-238, plutonium-239/240, americium-241, cesium-137, strontum-90, tritium, uranium-234, uranium-235, and uranium-238. Other elements such as barium, beryllium, calcium, chromium, cobalt, copper, iron, magnesium, manganese, nickel, potassium, sodium, vanadium, zinc, antimony, arsenic, cadmium, lead, selenium, silver, thallium, and mercury were also assessed. All radionuclides, with the exception of plutonium-239/240, americium-241, and cesium-137 were statistically similar ($p<0.05$) to regional background concentrations ($n=11$). The amounts of plutonium-239/240, americium-241, and cesium-137 in the whole body samples of field mice were far below screening levels and regulatory standards and are not expected to affect field mice population attributes. All other elements were similar to background. No increasing trends of any radionuclide or metal elements were noted. Levels of cesium-137 statistically decreased over time.

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Name: Andrew Gonzales
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School: University of New Mexico

Group(s): WX-**1**
Mentor: Edward Jacquez
Category: Information Technology
Type: Group Poster Presentation
LA-UR: 14-25945

Electronic Rounds-Keeping and Data Analysis

In order to increase the productivity of DARHT, an electronic data collection process will be implemented with the use of IPads. The IPads along with AuditMatic will provide a reliable, timely, and efficient method for conducting DARHT facility operational rounds. This system is designed to prevent data entry errors and provide trend analysis. IPads give the greatest mobility options for the operator while conducting rounds from room to room and when climbing ladders. The IPad will be carried by the DARHT Operators are conducting rounds with the use of AuditMatic. The operator will verify all equipment is in working order and tolerance within the specified limit. Once the operator rounds are completed, the operator will connect the IPads to the USB to Ethernet cable where the Automatic software will upload the information to the yellow net where that information will be used for trend analysis and record keeping.

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Group: OSH-OM
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Category: Health & Safety
Type: Individual Poster Presentation
LA-UR: 14-25746

Break Time Anytime

Sitting for 4 hours or more a day increases an individual's risk of sedentary health disorders and Musculoskeletal disorders. Luckily an individual can make a few changes in his/her workstyle to avoid certain injuries. A sit-to-stand desk, treadmill desk, standing/stretching breaks, and active standing breaks all help reduce injury to an office worker. The health effects of standing/stretching and active standing are the same. Treadmill desks do more for your body than a sit-to-stand desk but are not a replacement for diet and exercise program.

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Group: OSH-OM
Mentor: Cindy Lawton
Category: Health & Safety
Type: Individual Poster Presentation
LA-UR: 14-25769

Designing an Ergonomically Sound Glovebox Glove

Ergonomic injury and radiation exposure are two safety areas of special focus for the Plutonium Facility (TA-55) at Los Alamos National Laboratory (LANL). TA-55 employs the largest number of gloveboxes (GB) at LANL with approximately 6000 gloves installed. The current GB glove design dates back to the 1960's and is not based on true hand anatomy, which presents several issues: short fingers, inappropriate length from the wrist to finger webbing, nonexistent joint angles and incorrect thumb placement. These design flaws are directly related to elbow (lateral epicondylitis) and thumb (DeQuervain's tenosynovitis) injuries. The current design also contributes to increased wear on the glove, causing unplanned glove openings (failures) which put a worker at risk of exposure. A new glove design must incorporate the varied physical attributes of workers ranging from the 5th percentile female to the 95th percentile male. Anthropometric hand dimensions along with current GB worker dimensions were used to develop the most comprehensive design specifications for a new glove. Finger lengths and joint angles were the most crucial elements to the new design. Dimensions of the transitions between finger lengths were developed using a step up/step down method along with percentile data in order to encompass the greatest range of users. A hand surgeon from the University of New Mexico collaborated with the project to determine the most functional joint angles for a working hand. An engineer integrated the final dimensions into a 3D SolidWorks model, forming the basis for the new glove mold. The new glovebox glove will decrease strain and physical stress felt on the upper extremities of glovebox workers, as well as material strain on the glove itself. The ergonomically correct design will diminish the risk of injury, improve worker comfort and productivity, and reduce exposure concerns.

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Name: Maria Trujillo
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Group(s): TA55-DO
Mentor: Dianne Wilburn
Category: Health & Safety
Type: Group Poster Presentation
LA-UR: 14-25801

Environmental Compliance

Our poster educates viewers on the environmental laws that are in place here at Los Alamos National Labs. We show that these laws are used to protect the health and safety of all LANL employees. Along with that our presentation provides information on how to comply with these laws in a safe and reliable manner.

Name: Savina Dimitrova
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School: University of New Mexico
Group: OCIO-IS
Mentor: Dale Leschnitzer
Category: Information Technology
Type: Individual Poster Presentation
LA-UR: 14-25824

Probabilistic Risk Assessment and Design Optimization Using SAPHIRE

The Nuclear Regulatory Commission (NRC) established a software-development project for Idaho National Laboratory (INL) to create fault trees and calculate risks for system failures. In 1987, INL introduced SAPHIRE – Systems Analysis Programs for Hands-on Integrated Reliability Evaluations. Los Alamos National Laboratory's Risk Assessment (RA) Team utilizes Microsoft Excel for the modeling, calculation and analysis of risks of Attack Trees.

SAPHIRE, a risk assessment tool that visualizes cut sets and analyzes probabilistic events for system failures, was assessed for utilization by the Office of Chief Information Officer (OCIO) RA Team. The risks associated with the introduction of sophisticated mobile devices and ever-changing technology for the Enterprise, were computed using the LANL Risk Based Information Security Model; then, these calculations were implemented in relevant Attack Tree Modeling scenarios utilizing the vector graphic capabilities and Microsoft Excel's equations. SAPHIRE bridges the gap between stand-alone risk calculations and sets of system failures that result in overall failure. The INL's tool allowed for optimization of Attack Tree Modeling, reducing time and errors input into the Fault Tree logic. SAPHIRE was assessed by trial-and–error methods on the basis of functionality, responsiveness to system changes, and overall capability to analyze failure and success. Human reliability analysis and Rare Event Approximation quantification methods were used for the implementation of attack trees in SAPHIRE.

SAPHIRE proved to be a robust tool for the implementation and visualization of Attack Tree Methodologies, enhancing the Chief Information Officer (CIO) and Chief Information Security Officer's (CISO) decision-making process. The OCIO officials determined that SAPHIRE's Probabilistic Risk Assessment (PRA) approach conserved LANL resources and extended analysis into Attack Trees.

SAPHIRE streamlined Attack Tree creation and introduced vast improvements in interpreting risks with system failures for the purpose of protecting the confidentiality, guaranteeing the integrity, and maintaining the availability, of information at LANL.

Name: Joshua Garcia
Program: UGS
School: New Mexico State University
Group: DCS-ISS
Mentor: Nicolas Miller
Category: Information Technology
Type: Individual Poster Presentation
LA-UR: 14-25382

Wireless Networks

We were assigned a wireless laptop project within Occupational Medicine. The desired end result was a system in which four laptops would be granted machine-based encryption and signing certificates that could then be relayed via the Windows 7 wireless management interface to allow the devices on the yellow wireless network. The certificates were obtained from NIE and granted to the devices directly. Since exporting the information on a windows machine would result in a password being applied to each certificate, the certs were requested AND exported on an OS X machine. Entrust was completely omitted from the process to that multiple users at Occupational Medicine could use the devices.

Name: Cody Jackson
Program: GRA
School: University of New Mexico
Group: OCIO-IS
Mentor: Dale Leschnitzer
Category: Information Technology
Type: Individual Poster Presentation
LA-UR: 14-25585

Evaluating Cyber Security Policies Through Metrics

Metrics are an important part of any business structure. Metrics provide a framework for which we decide the success or failure of an operation, project, or system. Within the world of cyber security metrics have a high priority as it is the basis of continuous monitoring. The continuous monitoring system can be likened to an immune system. The first stage of an immunological response is identifying a threat or issue. According to the National Institute of Standards and Technology continuous monitoring is an integral part of the information security plan because it determines the ongoing effectiveness of security controls, policies, and standards as well as compliance with legislation and policies. Effective continuous monitoring involves the collection of data from every area of the information systems environment. In an environment as complex, diverse, and large as LANL this can present a difficult challenge. No single tool can be used to collect the required information; instead we must rely upon a number of individual tools. The challenge comes from combining the information into a useful collection. It is important that this data be collected and aggregated in a manner that allows a CIO or CISO to make decisions based on reliable and readable information. For the information to be used in timely decision making it should be aggregated into a dashboard. A dashboard provides important information aggregated to be read at a glance. This process is a balance between statistical science and graphical art.

Name: Toreelyn Murphy
Program: UGS
School: Indiana Tech
Group: IAT-4
Mentor: James Brooks
Category: Information Technology
Type: Individual Poster Presentation
LA-UR: 14-25197

Virtual Machines

Technology is a huge value to our country that continues at a startling rate. Many buildings have rooms full of servers upon servers, which create space issues, energy efficiency issues and can be very costly. To hold the amount of data we store could easily fill a room of servers; my solution this summer was to go virtual. I discovered that it was cost effective and more energy efficient to use what we call virtual servers. To put it into simple terms, a virtual server is a server built within another server. A virtual server is created on a physical box using software such as Hyper-V. It allowed me to create various servers without the unnecessary physical servers stacked ceiling high. This summer I was able to prove it to be more efficient and just as reliable as physical servers, and I didn't have the many amounts of physical servers like we have seen in past years. While on the virtual machines, I used IBM Domino to create and allow clients to access our databases via a client and/or the web. Using Domino I had created several domains that hold large amounts of databases that in return can be viewed or accessed as a website for the client's use. Using Domino I created several domains and cross-certified them, which allows for cross domain communication. These domains are the first step to creating a web site on the internet that you and I can access every day. In conclusion, during this summer I was able to build a total of six servers on only two physical servers and create and run four domains through Domino, that were able to communicate, replicate and store the databases.

Name: Simon Redman
Program: UGS
School: University of Utah
Group: ISR-3
Mentor: Scott Miller
Category: Information Technology
Type: Individual Poster Presentation
LA-UR: 14-25498

Driver Development and Data Acquisition on the SBC1651

ISR requires reliable, low-cost, low-power systems for data acquisition. One device which has been identified as a possible candidate is the SBC1651. This presentation will focus on my efforts to upgrade and improve this system by writing firmware to troubleshoot stability problems and software to harness its data acquisition capabilities, extend its functionality, and enable long-term support.

Name: Tanner Vaughn
Program: UGS
School: Colorado State University
Group: NEN-3
Mentor: Davis Thomson
Category: Information Technology
Type: Individual Poster Presentation
LA-UR: 14-25559

Commodity Fingerprinting for Identification of Strategic Goods

Aspiring proliferant 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 can also be of use in the development of WMD; these are known as "dual use" commodities. The proliferation of these commodities to entities that would likely use them for other than their non-commercial applications is prevented by adherence to international agreements in the form of implementation of legislation by various countries in response to UN Security Council Resolution 1540.

This poster gives a brief overview of how we traditionally teach enforcement officers to identify these commodities qualitatively as well as demonstrate the importance of a new method of quantitatively describing dual use commodities. Fingerprints are based on four quantitative parameters of the commodity: size, weight, cost, and typical shipment quantity. These fingerprints will augment the International Nonproliferation Export Control Program's curricula and will aid law enforcement in identification of strategic commodities.

Name: Madeline Barker
Program: GRA
School: University of Oregon
Group: MST-7
Mentor: Rob Gilbertson
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25395

Synthesis of Nanoscale Hollow Polymer Spheres

Hollow polymer nanocapsules are ideal candidates for inertial confinement fusion (ICF) experiments. ICF is monitored by X-ray imaging of targets to analyze the shockwave produced. The ideal target is low density and low Z so that it does not have a large effect on the radiation transport, but can still be imaged by X-rays. Ultra-low density foams, ρ = 25 mg/cc, fulfill this criteria. Hollow polymer nanocapsules with diameters of 200 nm would provide the desired density. To synthesize hollow polymer nanocapsules, monomers are loaded into the hydrophobic bilayer of a surfactant vesicle and polymerized by UV irradiation. Low polydispersity can be achieved by extruding the solution of catanionic surfactant vesicles and monomers before adding the photoinitiator. UV photopolymerization produces hollow spheres with 200 nm – 10 μm diameters verified by UV-Vis, DLS, and SEM.

Name: Mollie Bello
Program: GRA
School: University of Oregon

Name: Jennie Keller
Program: GRA
School: University of Oregon

Group(s): MST-7
Mentor: Zach Smith
Category: Chemistry
Type: Group Poster Presentation
LA-UR: 14-25491

Plackett-Burman Analysis of Syntactic Foams

Syntactic foams are an important category of composite materials that have abundant applications in a wide variety of fields. The current study utilized a Plackett-Burman experimental design to investigate the effects that seven predetermined variables would have on properties of syntactic foams filled with 3M™ glass microballoons. Findings from this investigation are meant to eliminate variables that don't significantly effect the properties of syntactic foams. Eight foam samples were created and tested using various characterization techniques. The data from these tests was then evaluated using a Plackett-Burman response coefficient calculation. This calculation was applied to determine the statistical significance of selected variables. Analysis of the results found three variables, matrix composition, THINKY mix rate and THINKY vacuum pressure could be eliminated as experimental parameters. These conclusions were based on physical measurements that showed drastic improvements in syntactic foam properties when one level of the variable was used over the other. Further study of these foams should maintain the effective levels of each eliminated variable while examining various ranges of microballoon distribution, microballoon density and microballoon volume fraction. Ultimately, this data can be used to design a detailed matrix of syntactic foams based on their microstructures. A matrix such as this can be used by clients to quickly identify which foam would best suit their application given one or two desired properties.

Name: Shanice Brown
Program: UGS
School: Prairie View A&M University
Group: MPA-11
Mentor: Cortney Kreller
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25426

The Effect of a Ceramic Overcoat on the Response of a Mixed-Potential Sensor

NOx sensing technology is being developed for application in vehicle emissions monitoring to improve fuel economy and monitor the NOx emissions in lean-burn and diesel engines. The NOx sensor described herein is a mixed-potential sensor that measures the non-nernstian potential of a mixture of gases. The NOx sensor is composed of La0.8Sr0.2CrO3 (lanthanum strontium chromite) and Pt electrodes with a YSZ electrolyte and a protective porous ceramic overcoat. The overcoat is used to protect the electrodes from containments such as heavy metals and water. The sensor response to 100 ppm of NO, NO2, NH3, C3H6, and C3H8 has been measured at temperatures ranging from 380 - 550° C. At the higher temperatures, it was observed that there was little to no response to the nitric oxides, but the sensor had a small but finite response to the hydrocarbons. As the temperature was lowered the response time decreased slightly, but it was observed that the response to all test gases, including the nitric oxides, had substantially increased. The NOx sensor with the overcoat is being compared to the NOx sensor without an overcoat to observe the response sensitivity to NOx. The effects of adding a Pt pre-catalyst to the overcoat on relative cross sensitivity will also be discussed. The purpose of adding the Pt pre-catalyst is to improve the gas selectivity. Ultimately, this will shift the relative selectivity by preferentially oxidizing the non-NOx species that the sensor is sensitive to, yielding a complete NOx sensor.

Name: Brie Buerkle
Program: GRA
School: University of Oregon

Name: Douglas Vodnik
Program: GRA
School: University of Oregon

Group: MST-7
Mentor: Markus Hehlen
Category: Materials Science
Type: Group Poster Presentation
LA-UR: 14-25392

Gaussian Modeling of Metal Foam Precursors

Nanoporous metal foams can be used in many applications. There are many methods of synthesis for metal foams, including combustion. Diammonium bistetrazolamine (DABTA) can be reacted with metals to form Me-BTA complexes, which can then be compacted into pellets and ignited with a hot wire or laser. Combustion occurs, which results in formation of N2 gas and the subsequent agglomeration of metal atoms into nanoporous foam. In order to investigate whether the proposed Me-BTA complex, TiBTA2, is the form present in the precursor solution its spectrum can be modeled in Gaussian and compared to the experimental spectrum.

Gaussian is a computational chemistry program which uses various quantum mechanical methods to predict properties of atomic and molecular systems. The theoretical methods used in this project were the Hartee-Fock (HF) method and the Density Functional Theory (DFT) method. Various basis sets were used, including 6-311G and LANL2DZ. Frequencies in the resulting spectra were scaled to match experimental data using established scaling factors.
Since BTA is a known compound, the fact that its experimental spectrum contained peaks at the approximate locations of the three major peaks in its computational spectra helped verify the reliability of the scaled computations. Conversely, the lack of a major peak in the experimental spectrum that exists in the computational spectra may indicate that TiBTA2 is not the correct form of the Ti complex present in the precursor solution. Alternatively, it may indicate that peak broadening effects were not taken into account in the computation. However, both the computational and experimental spectra may need to be refined and examined in greater detail before conclusions can be drawn. Regardless, more work is needed before rejection or confirmation of the presence of specific Ti complexes in the precursor solution can be determined.

Name: Olivia Dippo
Program: UGS
School: Carnegie Mellon University
Group: MST-8
Mentor: Veronica Livescu
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25664

Spallation in High-Purity Copper Under High-Explosive Shock Loading

Shock wave testing of metals is used to study extreme loading conditions which are of high engineering importance for defense applications in nuclear and non-nuclear weapons. As shock waves propagate through a material, release waves are generated from free surfaces. The intersection of these waves in a ductile material causes tensile stresses which can initiate void formation. Complete separation of the material, or spallation, can occur if the internal stresses are high enough. In some cases, free-surface velocity data can show a curve indicative of complete spallation, without visible post-mortem spallation in the material. In this case, it has been hypothesized that recompression occurs, closing the voids created by the initial shock. To investigate this, OFHC copper samples were shock-loaded using a Taylor wave generated with high explosives nitromethane (NM) and PBX 9501. Post mortem analysis of samples' cross-section indicates no evidence of recompression. Analysis of optical micrographs and electron backscatter diffraction images showed stronger plastic deformation in samples driven by PBX 9501 which has a higher rate of energy release. However, areas of damage exhibited strain localizations but grain boundaries across these regions were perfectly aligned and no cracks were visible. In addition, individual voids found along localization linkages keep their spherical shape. Such behavior would not be expected if sample was recompressed.

Name: Jason Guo
Program: UGS
School: Texas A&M University
Group: MST-8
Mentor: Osman Anderoglu
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25578

Metallurgical Characterization of a Railroad Spike

A railroad spike of unknown material was prepared and etched and the microstructure was characterized using Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), hardness testing and optical microscopy. From examining the composition of the unknown material, one can determine the elements that make up the steel used for railroad spikes. In this particular case, the spike contained a majority of iron with the second major element being carbon along with traces of silicon and nickel. This combination of elements yielded a hardness of an average of about 325 HV, a hardness strength greater than the average of regular steels. Furthermore, the microstructure was studied to determine what made the material exceptional.

Name: Simona Martin
Program: UGS
School: University of Chicago
Group: MPA-11
Mentor: Aditya Mohite
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25526

Characterizing Perovskite Crystallization for Photovoltaic Applications

This project aims to optimize the crystallization of perovskite, a substance with the potential to increase efficiency in photovoltaics, using various crystallization techniques. The techniques primarily used were spin-coating and dip-coating a lead-based perovskite solution onto substrates, which were then observed with various measurement techniques to characterize the crystals made. These crystals were furthermore observed to determine the ferroelectric properties of the substance, with the ultimate purpose of optimizing the efficiency of perovskite-based photovoltaics.

Name: Christina Hanson
Program: GRA
School: Massachusetts Institute of Technology
Group: MPA-CINT
Mentor: Jennifer Hollingsworth
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25287

Giant Quantum Dots: Stable and Efficient Emitters for Solid-State Lighting

The current push toward the implementation of Solid-State Lighting (SSL) as a more energy efficient solution for commercial and residential lighting applications has accelerated an interest in making light emitting diodes (LEDs) cheaper, more color and temperature stable, and with more color balanced optical properties. Recently, semiconductor quantum dots (QDs) have been proposed as a potentially 'earth abundant' and less costly alternative to the rare-earth phosphor down converters that are currently used in LEDs. Additionally, QDs allow for a broader range of color tuning both through broad excitation and sharp photoemission that can be tuned across the visible range. Specifically, our work focuses on the use of "giant" QDs (gQDs), core-shell QDs that have very thick shells that confine the holes to the core of the QDs and allow for the electron to be delocalized into the shell layers. These gQDs exhibit a large Stokes shift (energy separation between absorption and emission), suppressed blinking and Auger recombination, resistance to photobleaching and high QYs. The large Stokes shift is a key characteristic of these gQDs for down-conversion applications, as it greatly decreases the amount of self-reabsorption at nano-mesoscale interfaces and, thereby, significantly improves solid-state performance compared to conventional core/shell QDs. We explore here the feasibility of gQDs as down-conversion phosphors for LEDs by testing environmental stability and performance in 'real-world' relevant LED constructs, demonstrating methods for minimizing the impact of thermal quenching to produce record down-conversion efficiencies.

Name: Anna Scott
Program: UGS
School: Montana State University
Group: MST-8
Mentor: Kenneth McClellan
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25276

Accident Tolerant Nuclear Fuels

Certain catastrophic nuclear reactor events, specifically the 2011 accident at Japan's Fukushima nuclear reactor, have led to interest in the development of accident tolerant nuclear fuels. In addition to improving performance during accident conditions, promoting better economics and reducing environmental impact are also important development goals. To be attractive to future nuclear power plant operations, the fuels must be compatible with either current reactor designs or those that will be used in the near future. The new fuels must also be compatible with fabrication, transportation and storage systems. A fundamental principle of development is that any new fuel must at least meet current nuclear energy operations in terms of safety and economy.

In order to meet these requirements, multiple characteristics of potential fuels that drive developmental goals must be considered: isotropic properties, cycle length, fissile density, melting point, thermal conductivity, durability, ease of fabrication from UF6, and compatibility with other uranium fuels.

Based on preliminary findings, UN-U3Si5 and UN-glass are both potential accident tolerant fuel composites. Glass is promising because of its protective nature against water, steam and oxidation, ease of fabrication, self healing properties, reduced fission product and gas release, potential for built in burnable absorbers and potential for use in the modified-open fuel cycle via a dry reprocessing route. To more fully assess the potential viability of these fuels, a fabrication process is being developed to produce fuel composites suitable for fresh fuel property management and testing under irradiation in a nuclear reactor.

In my presentation I will review basic design and testing processes of new accident tolerant nuclear fuel composites as well as my progress in fabricating and testing specific nuclear fuel composites such as those mentioned above.

Name: Andre Spears
Program: UGS
School: Southern University and A&M College
Group: MPA-11
Mentor: Tommy Rockward
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25713

Investigating the Interactions of Competing Adsorbates on Pt Catalysts using Elect

We studied the interactions of carbon monoxide and hydrogen sulfide on Pt electrodes, in both isolated and combined experiments. This study utilized a 200:1 concentration ratio for CO and H2S, respectively. Such ratios are not uncommon in hydrogen fuel streams. Furthermore, we varied the time of exposure for each adsorbate to capture their signature oxidation peaks, and subsequently repeated the experiments with both species present. We show a direct correlation between the time of exposure and surface coverage by probing the chemisorption of CO and H2S and their subsequent oxidations for quantification. Our findings agree with previously reported PEM fuel cell results, in that the CO adsorption kinetics are faster but they form much weaker bonds with platinum surfaces.

Name: Matthew Ticknor
Program: HS COOP
School: Los Alamos High School
Group: MPA-CINT
Mentor: Jennifer Hollingsworth
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25288

Creating Designer Metal Arrays Using Nanosphere Lithography

The technique of nanosphere lithography was used to create well-ordered arrays of metal islands. This entailed first depositing onto a glass or silicon substrate hexagonal arrays of polystyrene (PS) micro-spheres (500-1500 nm in diameter) by self-assembly. The PS sphere layer was then used as an 'evaporation mask'. Metals were evaporated onto the mask. Most of the metal coats the PS spheres, but some passes through the spaces between the spheres, creating an array of metal islands where each island is comparable in size to the gaps between the PS spheres. In this project, metal island sizes and separation distances were tuned by changing the size of the PS spheres used to make the mask and by controllably melting the PS spheres to partially close the sphere-sphere gaps. Both aspects of the technique will be described here, as well as different approaches for sphere self-assembly, including air evaporation, vacuum-assisted evaporation, liquid-air interface assembly, and spin-coating. The approaches will be compared with respect to achieved large-area sphere ordering. Finally, we describe the two classes of metal arrays created using the PS sphere masks: magnetic and non-magnetic, low-melting metals. The former is used to realize new magnetic properties that can emerge when magnetic islands are assembled in arrays such that the islands interact and produce collective (coupled island-island) magnetic behavior. The latter low-melting-metal (e.g., bismuth, tin) arrays are used as growth catalysts for synthesizing semiconductor nanowires. The nanowires grow wherever there is a metal island, and in this way, the metal islands 'template' an ordered array of nanowires, which have applications in solar energy harvesting and as new light sources.

Name: Hsinhan Tsai
Program: GRA
School: University of New Mexico
Group: C-PCS
Mentor: Hsing-Lin Wang
Category: Materials Science
Type: Individual Poster Presentation
LA-UR: 14-25564

Designing High Efficiency OPV by Controlling the CT Rate at D/A Interface

Controlling and manipulating the charge transfer rate at the donor-acceptor interface is the essential key for achieving high efficiency organic solar cell (OSC). The overall power conversion efficiency in an organic solar cell depends on the balance between the rates of exciton dissociation, recombination and separation at the donor acceptor interface. Conventional bulk heterojunction solar cell architecture doesn't have a complete control over those rates at the interface. Here, we demostrated that we can manipulate the charge transfer rate at the P3HT/C60 interface by inserting a mono- and multi-layer of functionalized oligothoiphenes, which leads to a complete suppression in the exciplex (or charge transfer state) recombination. We observe that the photocurrent increases by 300 times, which in turn results in an increase in the overall power conversion efficiency by an order of magnitude. Moreover, we find that the oligothiophenes with an odd number of rings (ter and penta oligothiophene) exhibit a much higher increase in the photocurrent in comparison to the oligothiophene with an even number of rings (tetra oligothiphene). STM measurements reveal that the oligothiophene with odd and even number of rings differ in their ordering respectively, that has a big effect on the overall device performance. We also find that this ordering is highly dependent on the side functional groups in the oligothiophenes. The mechanism of photocurrent generation will be discussed and a simple transport model will be used to explain the change in the charge transfer and recombination rates and predict current-voltage curves.

Name: Alicia Dominguez
Program: UGS
School: University of New Mexico
Group: NEN-5
Mentor: Carolynn Scherer
Category: Mathematics
Type: Individual Poster Presentation
LA-UR: 14-25882

Distributed Security Framework for Modern Workforce

This poster considers the current challenges for nuclear security, and proposes a conceptual framework to address those challenges. There are several emerging factors that affect nuclear security:

1. Relatively high turnover rates in the nuclear workforce compared to the earlier years of the nuclear industry, when nuclear workers were more likely to have secure employment, a lifelong career at one company, and retirement on a pension plan.
2. Vulnerabilities stemming from the ubiquitous presence of modern electronics and their patterns of use by the younger workforce.
3. Modern management practices, including outsourcing and short-term contracting.

In such a dynamic and complex environment, nuclear security personnel alone cannot effectively guarantee adequate security. This poster proposes that one solution is a distributed security model in which every worker at a nuclear facility takes responsibility for sustaining the components of nuclear security.

Name: Duncan McGregor
Program: GRA
School: Oregon State University
Group: T5
Mentor: Gyrya Vitaliy
Category: Mathematics
Type: Individual Poster Presentation
LA-UR: 14-25956

M-adaptation for the Electric Vector Wave Equation

The efficient, accurate approximation of Maxwell's equations in the time domain has applications to a number of practical problems: particularly when signals have large bandwidth. Our equation of interest is second order formulation of Maxwell's equations where the signal is assumed to be constant in the z direction which we call the transverse electric vector wave equation.

Mimetic finite difference constructions do not produce a unique method. This non-uniqueness produces a family of methods which all have certain formal properties (like accuracy). This property can be exploited by parameterizing the family and selecting a member which is optimal with respect to some criteria, for example minimal phase error. This processes is called M-Adaptation.

We produce a four parameter MFD family which includes the lowest-order Nédélec edge elements as a member. The lowest order Nédélec method has second order dispersion error. By performing a discrete dispersion analysis for the family, we select a member which exhibits super convergence of the fourth order in phase error. We will present the numerical dispersion analysis of the family, construction of the optimal member, von-Neumann stability analysis and a selection of numerical demonstrations.

Name: Bridget Bohlin
Program: HS COOP
School: Santa Fe Prep

Name: Raquel Pacheco
Program: HS COOP
School: Espanola Valley High School

Group(s): XTD-PRI
Mentor: Leslie Sherrill
Category: Physics
Type: Group Poster Presentation
LA-UR: 14-25272

Sensitivity to Initial Conditions in Inertial Confinement Fusion Capsules

Inertial Confinement Fusion (ICF) is a type of fusion aimed at producing energy by using high-powered lasers to create fusion conditions in a fuel capsule. While nuclear fission creates radioactive waste, ICF produces practically none at all. It has the potential to become a very valuable energy source. Currently, the goal is still to produce more energy than is used. However, there are currently several obstacles standing in the way of producing a usable amount of energy. One major problem in ICF is the mixing that occurs between the comparatively cool outer layer of CH and the hot core of deuterium where the fusion transpires. Mixing lowers the temperature of the implosion core and decreases the total fusion yield significantly. It is thought that decreasing the amount of mix will be very useful in achieving energy output goals. This project was aimed at determining the initial conditions which ought to generate the least amount of mix. We ran simulations using a Lagrangian rad-hydro code called HELIOS, basing the setup on an experiment done at the OMEGA laser in Rochester, NY. Two main variables were tested: fill pressure and shell thickness. To test shell thickness, we ran simulations at a constant 20 atm and varied the shell thickness from 10-30 µm. To test fill pressure, we ran simulations using a constant 25 µm shell and varied the pressure from 15-30 atm. Since HELIOS does not calculate mix, we then post-processed the data obtained from HELIOS with a program which calculates the amount of mix in a given simulation. We show that ICF implosion cores are very sensitive to shell thickness but not to fill pressure.

Name: Matt Catlett
Program: UGS
School: Arizona State University
Group: P-24
Mentor: Eric Loomis
Category: Physics
Type: Individual Poster Presentation
LA-UR: 14-26102

Laser and Gas Gun Impact Experiments for Dynamic Material Property Measurements

The work performed this summer is in support for future Richtmyer-Meshkov instability and spall damage experiments at Los Alamos National Laboratory. The primary product will be a operational gas gun set up. A new target mount must be designed, fabricated and tested for the old gas gun system. The target mount design in conjunction with an alignment procedure must allow for high precision and repeatability in firing. The time of flight and firing jitter will be determined in addition to the production of pressure vs. velocity curves for a given projectile mass. Additionally, minor improvements can be made to the existing set up of the gun including: raising efficiency by removing a sharp turn in the gas flow path, extending the distance between the gun and the firing switch for safety, and minimizing the gun movement during firing. Finally, minor contributions to existing projects will be performed, including data analysis of TRIDENT laser experiments and the creation of MATLAB codes to test theoretical predictions vs. acquired data.

Name: Nico Cruz
Program: UGS
School: Indiana Univ.-Purdue Univ. Indianapolis
Group: EES-14/P-21
Mentor: Michael Malone
Category: Physics
Type: Individual Poster Presentation
LA-UR: 14-25181

Tracking Water Flow in Trees Using NMR

Water is a tree's primary resource. By measuring water flow in trees, we obtain a relative measure of the tree's health. To accomplish these measurements, we look to nuclear magnetic resonance. Though there are other methods of measuring a tree's water content, NMR is unique in that it can be made both non-invasive and portable. Traditional physiological methods normally involve changing the water content and flow through destructive operations, such as drilling, effects which we avoid completely due to the noninvasive nature of NMR. Over the span of several days, we measured the water flow in an aspen cutting, revealing how water consumption changes as a tree dies.

Name: John Goodell
Program: GRA
School: University of Maryland
Group: NEN-1
Mentor: Andrea Favalli
Category: Physics
Type: Individual Poster Presentation
LA-UR: 14-25881

Initial MCNP Simulations of Neutron Production at the Laser-Driven Neutron Source

Detecting shielded nuclear material en route remains a challenging task. The need is for a fast, movable, and operationally safe neutron source featuring energy tunable and high directional neutron fluence, overcoming the limitations of present methods, which typically produce isotropic monoenergetic neutrons. Recent experiments show that a short-pulse laser-driven neutron source possesses these features, allowing for the interrogation of variable shielding conditions and increased signal for the interrogation while improving operational safety. The short-pulse high-power laser is focused on a foil of deuterated plastic, creating an accelerated deuteron beam directed towards a neutron converter. The neutrons produced from various nuclear reactions have an array of energies dependent on the source properties. Neutron production from beryllium and copper converters is investigated using MCNP6 Monte Carlo transport code. For these preliminary simulations, two deuteron sources were modeled: a parallel beam and a more realistic cone with a vertex angle of 40 degrees, for energies from 10-200 MeV. Simulations show that the parallel beam provides the most ideal results, while a simple cone shows significant deviations from ideal. Both types emit neutrons anisotropically, with a distinct energy peak in the forward direction. This neutron energy peak generally is approximately half of the source energy. Neutron fluence is highest for small dispersions about the beam axis and decreases at wider angles. The percentage of forward directed neutrons is 60-85%, depending on the particular source/converter combination. Of these forward neutrons, 2-15% are within 10 degrees of the beam axis. Total neutron yield increases quadratically with the source energy for all source/converter combinations until the deuteron range exceeds its path through the converter. After this point, neutron production plateaus. Beryllium typically yields more desirable results than copper. The directionality and energy selectivity of this neutron source are highly desirable for neutron interrogation applications.

Name: Lauren Marus
Program: GRA
School: Colorado School of Mines
Group: C-IIAC
Mentor: Francois Nortier
Category: Physics
Type: Individual Poster Presentation
LA-UR: 14-25329

Proton Beam Energy Characterization

Protons generated in an accelerator can be deposited in target materials producing a large inventory of radioisotopes useful for medical treatment procedures and many other applications. Accurate characterization and control of the energy of the proton beam is crucial for optimizing isotope production schemes and performing accurate research. Most beam energy monitoring systems are limited to measurements far upstream of a target or are prohibitively invasive for some facility designs.

We describe our attempts to measure and simulate the proton beam energy incident on production targets and experimental research foils at Los Alamos' Isotope Production Facility.

In order to characterize the beam energy, we employ several techniques including experimentally measuring isotopic ratios, using monitor foils in thin foil stacks, and a performing a direct time-of-flight measurement. These methods, combined with computational simulations, paint a clearer picture of the beam conditions. These techniques reinforce one another, effectively building confidence in a toolbox for assessing the beam. Confidence in computational simulation is crucial to the accuracy of cross section measurements, optimizing isotope production targets, and defining a limit where simulations are most accurate.

Name: Brandon Medina
Program: UGS
School: NM Tech
Group: P-23
Mentor: Brenda Dingus
Category: Physics
Type: Individual Poster Presentation
LA-UR: 14-25602

HAWC: The High Altitude Water Cherenkov Detector

The High-Altitude Water Cherenkov (HAWC) observatory is a wide field-of-view detector sensitive to gamma rays of 100 GeV to a few hundred TeV. Located in central Mexico at 19 degrees North latitude and 4100 m above sea level, HAWC will observe gamma rays and cosmic rays with an array of water Cherenkov detectors spanning approximately 22000 square meters, with each Cherenkov detector being comprised of 3 peripheral and 1 central photomultiplier tube (PMT) at the bottom of a tank. The completed 300 tank HAWC array is scheduled to be operational by the end of 2014.

This presentation will serve as a synopsis of the work that I have contributed to the project this summer. In particular, I will be discussing analyses that I conducted on the characteristics of the PMTs, as well as the electronics that are associated with recording the data produced by the PMTs. Precise measurements of the characteristics of the PMTs and the electronics is necessary for correct reduction and interpretation of the HAWC data. My analyses are based on investigations using the LANL setup of the HAWC electronics, and my results will serve as a verification of our understanding of the HAWC detector.

Name: Benjamin Schilling
Program: UGS
School: New Mexico Tech
Group: WX-9
Mentor: Dana Dattelbaum
Category: Physics
Type: Individual Poster Presentation
LA-UR: 14-25479

Electromagnetic Multiple Shock Tracker Gauges

Electromagnetic particle velocity gauges were developed and have been used at Los Alamos National Laboratory since the 1980's. The gauges are used at Los Alamos to study the initiation behavior of explosives under various conditions. All the experiments which use electromagnetic particle velocity gauges are designed to be one dimensional so that the shock wave can be characterized by the gauge technique. Arnaud Sollier, who works for the CEA (French Alternative Energies and Atomic Energy Commission), is fielding LANL electromagnetic particle velocity gauges in his experiments to see if the gauges can be used to characterize multi-dimensional reactive flow. Sollier found that curvature has a pronounced effect on the gauges. Sollier's experiments lead to the development of a multiple shock tracker gauges, with all the shock trackers aligned to the same reference line. These new gauges have been successfully tested in initiation and steady detonation conditions.

Name: Stephen Taylor
Program: UGS
School: University of Wisconsin, Madison
Group: P-24
Mentor: Thomas Weber
Category: Physics
Type: Individual Poster Presentation
LA-UR: 14-00009

Determination of Plasma Density and Speed Using Transverse Interferometry

The Magnetized Shock Experiment (MSX) is studying the physics of super-critical magnetized shocks by accelerating a Field Reversed Configuration (FRC) plasmoid to high velocity and then stopping the FRC with a static magnetic field. FRCs are compact toroidal equilibria with no toroidal field and high average plasma β. FRCs can be translated in a linear vacuum system between the formation theta coil to the stagnating magnetic field. Knowing the plasma density and speed is crucial for establishing the conditions for shock formation. A two-cord transverse interferometer system has been built to quantify the plasma's density profile and speed as it travels down the machine axis. Line integrated density profiles and velocity measurements will be presented.

Name: Christopher Triola
Program: GRA
School: College of William and Mary
Group: NSEC
Mentor: Alexander Balatsky
Category: Physics
Type: Individual Poster Presentation
LA-UR: 14-25909

Many-Body Instabilities and Mass Generation in Slow Dirac Materials

In conventional materials the importance of Coulomb interactions for determining the electronic ground state is dependent on the density of the electrons and is thus a tunable parameter. In contrast to this, the importance of coulomb interactions in Dirac materials is a characteristic of the system depending largely on the material's Fermi velocity that determines the kinetic energy. Thus the relative strength of Coulomb interactions in Dirac materials is not easily tuned. In previous studies no conclusive experimental results have been able to show the existence of an interaction-driven gap. This implies that the kinetic energy of carriers in these systems is too large to permit ground states with interaction induced gaps. However, there are reasons to suspect that the surface states hosted by topological Kondo insulators can be described as massless slow Dirac fermions with much smaller Fermi velocity than previously studied systems, a direct consequence of f-electron physics in these materials. We investigate the effect of electron correlations and show that Coulomb interactions will play a major role in determining the ground state of these slow Dirac materials. One material predicted to fall into this class is plutonium hexaboride, PuB6. The topological nature of the Kondo insulating state will produce surface Dirac excitations with very small Fermi velocity on the scale of 10% of regular Fermi velocities seen in metals. Therefore, we propose to look for the gapped states on surfaces of PuB6. This work advances the field of Dirac materials and enriches our understanding of the f-electron physics in actinide-based materials.

Name: Matthew Tyson
Program: UGS
School: Furman University
Group: MPA-CINT
Mentor: Richard Sandberg
Category: Physics
Type: Individual Poster Presentation
LA-UR: 14-25421

Lensless Microscopic Imaging Using a Tabletop He-Ne Laser

As scientific understanding developed at scales far beyond the capabilities of the human eye, microscopy emerged as a powerful tool for studying the structural composition of materials and biological specimens. As such, microscopy provides the foundation for progress in a myriad of scientific fields. The primary goal with regard to microscopy is to develop an ideal microscope—one capable of producing high-resolution images of nanoscale samples with femtosecond time intervals. Pulsed x-ray sources present a promising method for high-speed, high-resolution imaging, though lenses compatible with these sources are difficult to make and inefficient. These issues can be avoided by an alternative to lens-based microscopy, a technique called lensless imaging or coherent diffraction imaging. Using this technique, the resolution of the reconstructed image is limited only by the illuminating flux on the sample and the wavelength of the illuminating source. In coherent diffraction imaging (CDI), a highly coherent source, such as an optical laser or x-ray free electron laser (XFEL), is focused onto an isolated sample and the resultant diffraction pattern is captured by a charge-coupled device (CCD) camera in high-resolution. The diffraction pattern is run through an algorithm that uses Fourier Transforms to recover phase and amplitude information, reconstructing a high-resolution image of the sample over numerous iterations. We demonstrate a tabletop, helium-neon laser based, lensless microscope suitable for undergraduate teaching laboratories.

Name: George Fleming
Program: UGS
School: University of Texas at Dallas

Name: Edgar Ronquillo
Program: UGS
School: Northern New Mexico College

Group(s): CCS-7
Mentor: Christine Sweeney
Category: Computing
Type: Group Poster Presentation
LA-UR: 14-25649

A Low-Cost Technique for Power Measurement of Computer Components

In recent years, power consumption in large computing platforms has become a great concern for research facilities requiring high performance computing. To address this growing concern, computer scientists and engineers have explored numerous solutions to optimize system performance while reducing overall energy requirements. The Department of Energy has been focusing on specific methodologies that would aid in lowering the overall energy footprint of these large platforms. One such focus is determining how varying programming approaches compare in terms of both performance and overall system power consumption. Power models developed by the department require accurate verification through simple high-speed, high-resolution power monitoring techniques. Microcontrollers were assessed as one such viable option that meet those performance criteria. The utilization of these boards combined with an array of shunt resistors and instrumentation amplifiers provides a low cost avenue for tracking power expenditure amongst individual components in a small computing platform. Data records from the sensors were collected and stored during specific runtime operations of scientific applications.

Name: Hailey Cambra
Program: UGS
School: Worcester Polytechnic Institute
Group: B-11
Mentor: David Fox
Category: Biosciences
Type: Technical Talk
LA-UR: 14-25760

Metabolic Engineering of Photosynthetic Bacteria for Biofuel Production

To alleviate our current dependency on fossil fuels, it is necessary to integrate the production of biofuels from renewable sources as a replacement for petroleum derived fuels into existing oil refinery infrastructure to maintain current and future energy demands. The green microalga species Botryococcus braunii Race B is able to generate large quantities of high energy density hydrocarbons called triterpenoids, which can be used as a replacement for petroleum sources. Specifically, this compound can be hydrocracked into gasoline; however, the slow growth of the microalgae inhibits its commercial viability. The ability of photosynthetic organisms to sequester CO2 makes such organisms more preferable for biofuel production, thus our team is working towards genetically engineering the faster growing cyanobacteria species Synechococcus elongatus PCC 7942 with genes from B. braunii Race B to exploit the metabolic networks in the cyanobacteria and produce the triterpenoids in a commercially viable way. To this aim we have constructed a DNA vector for insertion to achieve high level expression in S. elongatus, and are using it to overexpress triterpene methyltransferase-1 (TMT-1), which converts naturally produced squalene into its dimethylated products. The overexpression of this enzyme has the possibility of creating a “metabolic sink” for the production of triterpenoids, should we observe a successful double homologous recombination event. Simultaneously, we are verifying TMT-1 is active when overexpressed in Escherichia coli using a coupled S-adenosylmethionine (SAM)-dependent activity assay, which allows us to predict the protein’s compatibility within a prokaryotic environment in a timely manner, as its rate of growth exceeds that of S. elongatus. We are also developing a High Performance Liquid Chromatography (HPLC) protocol to detect dimethylsqualene to rapidly screen for product once a successful genetically modified cyanobacterium is isolated and characterized.

Name: Shailja Jakhar
Program: GRA
School: Saint Louis University
Group: C-PCS
Mentor: Harshini Mukundan
Category: Biosciences
Type: Technical Talk
LA-UR: 14-25497

Integrative Bio Surveillance

Our project is aimed at achieving integrative bio surveillance, which is the integration of clinical, meta, diagnostics and pathogen characterization data, to improve public health outcome and facilitate predictive epidemiology to inform on emerging infections. The study is based on a pediatric population in Siaya, Kenya, where the children are inflicted with diseases such as malaria, bacteremia associated with pathogens such as Salmonella, Staphylococci, and Streptococci. Clinical and meta data has been collected from a cohort of over 1600 patients in the last 12 years by our collaborator, Dr. D. J. Perkins. However, accurate diagnostics and pathogen characterization is required to analyze emerging infections. To achieve this, we propose to integrate this information with novel diagnostics and pathogen characterization data generated using LANL technology and capabilities. We have already developed rapid fieldable diagnostic assays and PCR-based assays for Staphylococci, Salmonella and Mycobacteria, and anticipate expanding to other pathogens like Streptococci. We have also been obtaining sequencing data for the isolates from Siaya, and integrating all this information into an epidemiological model. My research is focused on circulating strains of Streptococci in Kenya, and current diagnostic strategies for their detection. Information on potential biomarkers that can be studied to develop techniques for detection of pathogen, incidence information, drug resistance strains of Streptococci, sequencing studies done so far, and available antigens-antibodies, was collected as a part of this project. A comprehensive report was prepared to inform the team on specific aspects of interest for further development of assays and models. In addition, I learnt to develop and validate fieldable assays for the pathogens using novel transduction mechanisms on a waveguide-based biosensor platform developed at LANL. I hope to continue work on the development of assays for Streptococci in clinical samples as a part of my Master's thesis in Public Health.

Name: Steven Liaw
Program: UGS
School: NMSU
Group: B-10
Mentor: Jun Gao
Category: Biosciences
Type: Technical Talk
LA-UR: 14-25554

Develop Multiple Applications using Ultra-High Throughput Droplet-Based Microfluid

The growing interdisciplinary field of droplet microfluidics has many applications within biological sciences. Much like how computers have advanced to fit into your pocket many laboratory experiments can be downscaled significantly because of this relatively new technology. Droplet based micro fluidics is done on a "lab on a chip device"- just like the name implies-it combines many laboratory functions onto a small device composed of channels; these devices will require less reagent, less sample size and, less lab equipment to be able to run a faster bioassay. These microfluidic devices exploit fluid physics and a pump system to form droplets with encapsulated cells and/or chemical reagents for biology and chemistry study. This ultra-high throughput droplet generator can generate ~5000 droplets/sec with picoliter size. With the amount of droplets formed, large scale bioassays are possible. Currently we developed many applications using this platform, such as single-cell/bacteria encapsulation, protein crystallization and nanomaterial crystallization.

Name: Timothy Sanchez
Program: GRA
School: The University of New Mexico
Group: B-11
Mentor: Srinivas Iyer
Category: Biosciences
Type: Technical Talk
LA-UR: 14-25530

Omic Analysis for Toxicology

Quantum dot (QD) nanoparticles have shown great potential for use as drug delivery, diagnostic, and imaging agents in biomedicine and as semiconductors in the electronics industry. QD biocompatibility can be easily altered by surface modification, such as conjugation and capping with biomolecules and polymers. In this study, we examined the effects of different QDs using a 3D in vitro human bronchial airway tissue model and human normal bronchial epithelial (NHBE) cells. Bronchial tissues and NHBE cells were exposed to QDs conjugated with polyethylene glycol (PEG), and terminated with various functional groups: 3nm CdSe-PEG-OCH3 (neutral charge), 3nm CdSe-PEG-COOH (negatively charged), 3nm CdSe-PEG-NH2 (positively charged). Our goals were twofold: first, identify endpoint cellular responses including the effects of QD charges on cell viability and oxidative stress by cellular assays, and second, identify more silent, sublethal effects in terms of biological functions and toxicities as well as potential long-term diseases/disorders by examining global protein expression profiles using proteomic analysis. . Proteomic analysis identified of 247 proteins was significantly expressed, of which 106 differentially expressed (>+ -2-folds). IPA analysis showed that cell cycle abnormalities, necrosis and cell death, protein synthesis and degradation were significantly affected, particularly in the lung tissues exposed to the negatively charged QDs. IPA analysis also predicted potential long-term effects including cancer, dermatological diseases and conditions, gastrointestinal disease, neurological disease and respiratory disease. These results from the proteomic analyses are consistent with the observed cellular responses and provide a molecular basis to understand the mechanism underlying the toxic effects of functionalized QDs, in physiologically relevant human model systems.

Name: Jeffrey Sward
Program: UGS
School: The University of New Mexico
Group: B-10
Mentor: Jun Gao
Category: Biosciences
Type: Technical Talk
LA-UR: 14-25555

Using a Microfluidic Approach to Analyze Bacteria Growth and Antibiotic Response

Many groups throughout the United States and the rest of the world are using microfluidics to increase the accuracy, repeatability, and speed of biological experiments. Using some of these newly developed microfluidic techniques, we have begun to construct the fairly large setup characteristic of microfluidics. We have also have begun work on designs to analyze how a well-established colony of bacteria reacts to antibiotics. This process includes device design using SolidWorks, fabrication of the devices using a soft lithography approach, device testing, and finally testing using green fluorescence protein (GFP) expressing bacteria specimens. Our data suggests that the bacteria growth and their antibiotic resistance /susceptibility can be precisely monitored in the defined micro-channels. We also observed that micron size channels can significantly alter the bacteria colonic morphology. Currently, we are also developing the ability to use more advanced microfluidic fabrication techniques as well as valve controllers and software to drive the valves. These systems utilize more cutting edge microfluidic designs, and could potentially improve both our experiments and analysis. In our future study, we will integrate automated microfluidic solenoid valves to control the antibiotic gradients to investigate the bacteria resistance and susceptibility.

Name: Louis Tkach
Program: UGS
School: University of New Mexico
Group: B10
Mentor: Jun Gao
Category: Biosciences
Type: Technical Talk
LA-UR: 14-25676

Microfluidic Design and Manufacture Using Laser Engraving & Cutting Technology

The intent of this project is to establish microfluidic fabrication capabilities using CO2 laser engraving and cutting technology at Bioscience Division (LANL). The fabrication process includes CAD design, laser-based manufacturing and device functional evaluation. The fabrication process is based off general engineering design processes: a preliminary design phase and concurrent design phases. This foundation included an identification of goals and requirements (functionalities), constraints, and by what means (specifications/parameters) we intend to reach the final goals and requirements. Accordingly, concurrent design phases follow initial device manufacture, assembly and functional evaluation with the purpose of optimizing the original or previous designs, thus, allowing for alternative approaches to reach expected functionality. Hence, post CAD design, manufacture, and assembly of microfluidic devices using laser engraving machine, evaluations of the properties of the device were performed. Evaluations of the properties of such devices included: material compatibility, filtration-mass retention in column, percent volume of elute in column, and a maximum elution rate. Thus, in conjunction with applying this design process we have been able to manufacture microfluidic devices for specific projects that meet expected functionalities such as integrating micro-columns into microfluidic device for tracing element analysis. This workflow enables the simplification of complex integrated functional microfluidic systems with expected requirements during the fabrication process.

Name: Joseph Macor
Program: GRA
School: University of Illinois, Urbana-Champaign
Group: C-IIAC
Mentor: Stosh Kozimor
Category: Chemistry
Type: Technical Talk
LA-UR: 14-25623

Selective Extraction of Minor Actinides with Heterocyclic Dithiophosphinic Acids

Nuclear energy will remain an important alternative to the combustion of fossil fuels until effective, renewable energy technologies can be realized on the large-scale. However, significant environmental and safety challenges remain with the processing and management of nuclear by-products, particularly for the transuranic actinides. A major bottleneck for the development of an efficient closed nuclear fuel cycle lies in the separation of minor actinides (MA = Am, Cm) from trace lanthanides (Ln) found in the spent fuel. Because trivalent 4f-Ln and 5f-MA exhibit nearly identical chemical and physical properties, efficient separation of the two remains a significant challenge in inorganic chemistry.

Despite these limitations, certain "soft-donor" ligands such as dithiophosphinic acids (R2PS2H, in particular where R = o-CF3Ph) have shown promise in the selective chelation of MA over Ln. Preliminary DFT calculations and sulfur K-edge XAS experiments have found a correlation between extractant selectivity and orbital overlap of the arene pi system and the PS2 core. In light of these findings, it was predicted that an optimal molecular geometry for the mixing of these orbitals would be attained via synthetic tethering of the aryl rings, and thus may afford an unprecedented affinity for the selective binding of actinides. The synthesis of a series of novel heterocyclic dithiophosphinic acids, K-edge XAS measurements, and performance in Eu/Am liquid-liquid extractions will be discussed.

Name: Raymond Hendon
Program: GRA
School: Middle Tennessee State University
Group: Xcp-8
Mentor: Scott Ramsey
Category: Computing
Type: Technical Talk
LA-UR: 14-24338

Conduction Invariance in Exact Solutions for Compressible Flow Code Verification

In 1991, S. Coggeshall1 published a series of 22 closed-form solutions of the Euler compressible flow equations with a heat conduction term included. A remarkable feature of some of these solutions is invariance with respect to conduction; this phenomenon follows from a subtle ancillary constraint wherein a heat flux term is assumed to be divergence-free. However, the conduction invariance property has been a key verification challenge in numerical simulation of these solutions. In this work, the discrepancy is resolved by recalling a well-known result from classical electrostatic theory: applying a divergence operator to the heat flux distributions exhibited by many of the supposedly conduction-invariant Coggeshall solutions yields a Dirac delta function source term instead of identically zero. Numeric simulation of these solutions including the delta function source terms show marked improvement in accuracy near the origin but are limited by the current energy source function capabilities of simulation software.

Name: Arley Schenker
Program: UGS
School: Carnegie Mellon University
Group: CCS-3
Mentor: Steven Brumby
Category: Computing
Type: Technical Talk
LA-UR: 14-25529

Computer Vision Algorithms for Labeling Social Media Video

Sparse representations of images have been used in computer vision algorithms to produce state-of-the-result classification results, and this technology is rapidly being adopted across both academia and industry (Google, Facebook). The academic state-of-the-art is to apply these algorithms to still images, but most of the visual data on the internet is in the form of video. In this experiment, we implement sparse representations and train a deep learning convolutional neural network to recognize objects in Twitter Vine videos. We examine speed of classification and accuracy, with training provided by the academic Image-Net crowd-source-labeled dataset. We apply our models to a validation set of Vine videos that have been classified manually.

Name: Benjamin Turrubiates
Program: UGS
School: New Mexico Institute of Mining and Tech
Group: HPC-3
Mentor: Jennifer Green
Category: Computing
Type: Technical Talk
LA-UR: 14-25630

Auto-Generated ClusterWide Configuration Tool

Modern HPC platforms are continuously increasing in processing ability to match the computational needs of the scientific community. Due to the high degree of reliability and performance that is expected from these platforms, correctness testing and performance base-lining are more important than ever. This sort of large scale testing can quickly become tedious if the task is not automated. A solution being developed is the Pavilion HPC Test Harness. The Pavilion project aims to ease the use and extensibility of test automation tools. One method of aiding ease of use is by providing an automated configuration utility. To ensure that the data collection scales efficiently we have implemented the tool using a parallel framework called the Component Based Tool Framework.

Name: Carlos Biaou
Program: GRA
School: University of Maryland, College Park
Group: P-21
Mentor: Chad Olinger
Category: Earth and Space Science
Type: Technical Talk
LA-UR: 14-25480

Improving Modeling of Solar Wind Ion Implantation

The Genesis mission was launched in August 2001 to collect samples of solar wind and return them to Earth. Thorough analysis of the solar wind in four regimes (Slow, Fast, Bulk, and Coronal Mass Ejection) revealed the concentration profiles of several elements in the periodic table in different target materials (Si, Au, DLC…). After the hard landing of the Genesis spacecraft, the targets were contaminated and the analysis was then heavily impacted. SRIM (Stopping and Range of Ions in Matter), a Monte Carlo based software, became extremely useful in constructing simulated concentration profiles and correcting them for contamination and backscattering through post-processing. To better match simulated and measured profile, a diffusion based approach was explored for hydrogen and deuterium. The approach seems promising but raises some questions in its effectiveness in accurately modeling the implanted ions.

Name: Sean Dolan
Program: GRA
School: University of Oklahoma
Group: ENV-ES
Mentor: LeAnn Purtzer
Category: Earth and Space Science
Type: Technical Talk
LA-UR: 14-25371

Obsidian Procurement and Social Interaction on the Pajarito Plateau A.D. 1200-1600

One of the missions of the Los Alamos National Laboratory's Cultural Resource Team is to document and protect archaeological sites located on the Lab's property that spans 7000 years of human occupation and cultural activity. The ancestral Puebloan's who lived here valued obsidian, a volcanic glass, because it was one of the preferred raw materials to make projectile points and other stone tools due to its sharp cutting edges, availability, and translucent color. Archaeologists can obtain the unique chemical signature of individual obsidian flows throughout the North American Southwest, including the nearby Jemez Mountains using geochemical X-ray fluorescence (XRF) analysis on the trace elements of obsidian to answer questions about ancient human behavior. In this presentation, I use XRF data from The Land Conveyance and Transfer Data Recovery Project (LA-UR-07-6025) and other projects in Bandelier National Monument to examine how obsidian procurement can be used to expound upon social dynamics behind the migration of people from the Mesa Verde region in southwestern Colorado into the Pajarito Plateau starting in the late 13th century. To do this, I incorporate a large sample size of sourced obsidian artifacts into Geographic Information Systems (GIS) to investigate social interaction, land use patterns, and diachronic patterns of obsidian procurement from A.D. 1200-1600. Results indicate that people through time and across space in the Pajarito Plateau used different obsidian sources and procurement strategies. I argue this occurred because of changes in settlement patterns, land use strategies, and social negotiations with incoming groups from Mesa Verde and the surrounding area during this time. This research contributes to the archaeology on LANL's property since it enhances our understanding of ancient social interaction and obsidian procurement through time on the Pajarito Plateau to make better assessments of archaeological data for future investigations and research questions.

Name: Beth Boardman
Program: GRA
School: University of California San Diego
Group: AET-5
Mentor: Troy Harden
Category: Engineering
Type: Technical Talk
LA-UR: 14-25445

Optimal Kinodynamic Motion Planning in Environments with Unexpected Obstacles

This paper presents and analyzes a new algorithm, the Goal Tree (GT) algorithm, for motion planning in dynamic environments where new unexpected obstacles appear sporadically. The GT builds on the RRT* algorithm by employing an initial RRT* tree rooted at the goal. When finding new obstacle information, O, the GT quickly constructs a new tree rooted at the current location of the robot, xI, by sampling in a strict subset of the free space. The new tree then reuses branches from the original tree so that it can produce paths to the goal. Compared to running the RRT*, the GT reduces, on average, the time needed to produce a path of equal cost. We prove that, generically, there exists a region, which is a strict subset of the free space, which can be used with the GT algorithm to produce a asymptotically globally optimal path. This region is theoretically characterized for planning problems in d dimensional environments. An alternative region is provided for robot with Dubins' vehicle dynamics and a vehicle with no dynamics both under a Euclidean distance cost function. Simulations for a Dubins' vehicle robot verify our results.

Name: Kimberly Clark
Program: GRA
School: University of Nevada Las Vegas
Group: XCP-3
Mentor: Avneet Sood
Category: Engineering
Type: Technical Talk
LA-UR: 14-25662

Characterization of the NPOD3 Detectors in MCNP5 and MCNP6

While the behavior of a critical nuclear system is easy to predict because it is in a steady state, a subcritical system is rather difficult to simulate because it exhibits time dependence and statistical fluctuations. Several Monte Carlo particle transport codes are capable of simulating subcritical systems. Two such codes are Los Alamos National Laboratory's MCNP5 and MCNP6 (Monte Carlo N-Particle) codes. Many years ago, an in-house patch was developed for MCNP5 to produce list-mode data (time and location of neutron absorption within a detector) to compare to the detector output for multiplicity measurements. Now that MCNP6 has replaced MCNP5 as the production code, it was necessary to determine whether MCNP6 was capable of providing list-mode data without the need for a patch.

Researchers performed a series of measurements in May 2012 to characterize the NPOD3 detector systems. The detectors were placed in varying states of disassembly to determine the effect of individual components on the detector response. The Los Alamos BeRP Ball was used as the SNM source in both a bare configuration and reflected by varying thicknesses of polyethylene (HDPE). A set of MCNP5 with the list-mode patch and MCNP6 simulations matching the experimental setups for the bare and reflected cases were run and the calculated list-mode data were compared to the measured data. The singles and doubles count rates and the leakage multiplication results show that both MCNP5 with the list-mode patch and MCNP6 adequately replicate the measurements. The advantages and limitations of each code for the use of obtaining list-mode data are explained.

Name: Leslie Kerby
Program: GRA
School: University of Idaho
Group: XCP-3
Mentor: Stepan Mashnik
Category: Engineering
Type: Technical Talk
LA-UR: 14-25560

Intermediate-Energy (> 1 MeV) Cross Section Models in CEM and MCNP6

The Cascade Exciton Model (CEM), version 03.03, is the event generator used in MCNP6 for collisions in the energy range of several tens of MeV to several GeV. CEM derives its inverse cross sections from reaction cross section models. These inverse cross sections are used to predict the production and emission spectra of nucleons and light fragments (up to Mg-28) in the preequilibrium and evaporation stages of a nuclear reaction. The current cross section models used in CEM03.03 are based upon the Dostrovsky model. Other cross section models, such as those developed at NASA, as well as Barashenkov and Polanski, are shown to be superior. Results of implementing the NASA model into CEM are given. Implications for MCNP6 are discussed.

Name: Jonathan Madsen
Program: GRA
School: Texas A&M University
Group: XCP-3
Mentor: Steven D. Nolen
Category: Engineering
Type: Technical Talk
LA-UR: 14-26040

Shared Memory Parallelism of MCATK with Minimal Locking Synchronization

Monte Carlo particle physics codes traditionally use distributed memory parallelism via message-passing interfaces (MPI) to produce run-time speedup on multiple processors. The distributed memory parallelism is generally implemented in a domain-decomposed fashion and/or a particle-decomposed fashion. The most common implementation for both is for each processor to have its own copy of the entire problem, leading to a linear increase in memory with respect to the number of processors. In domain-decomposed, each processor works on specific spatial section of the problem. In particle-decomposed, each processor works a subset of the particles of the problem. The shared memory parallelism model generally eliminates the increase in memory consumption but introduces a unique challenge in reproducibility, as the order of operations are non-deterministic, and threads must be synchronized to ensure read and write operations on data are not in conflict with each other. The Monte Carlo Application Toolkit (MCATK) is capable of both domain-decomposed and particle-decomposed distributed memory parallelism via MPI and now features particle-decomposed shared memory parallelism using the Intel Thread Building Blocks (TBB) library. For optimal CPU and wall-clock speedup, locking synchronization via mutexes is avoided almost entirely throughout the code, with the primary exception of memory operations on the global storage container for the particles, through the use of atomics (with C++11, Boost, or TBB atomics implemented to share a common interface) and a complete re-write of the STL deque template class using a custom allocator to handle atomics. These implementations are necessary because traditional STL container make ample use of the copy constructor for the template data type and the copy constructor for atomics is not valid. Scaling studies on CPU speedup, wall-clock speedup, virtual memory usage, RAM usage, and solution difference with respect to the serial implementation are provided.

Name: George McKenzie
Program: GRA
School: University of Illinois
Group: NEN-2
Mentor: William Myers
Category: Engineering
Type: Technical Talk
LA-UR: 14-25880

Rossi Alpha Method

The Rossi Alpha method determines the prompt neutron decay constant in a nuclear fissioning system at or near delayed critical. The prompt neutron decay constant is an important parameter to know for a critical assembly because it is a major contributor to the dynamic system behavior. The Rossi Alpha method consists of an experiment designed by Bruno Rossi in the 1940's and a heuristic model of the neutron population in a chain reaction concurrently developed by Richard Feynman. The experiment utilizes the fact that neutrons in a fission system occur in chains and not as single entities. The experiment is designed to measure the correlation between neutron counts. Feynman's equation statistically separates the neutron counts into accidental or correlated neutron pairs based on the time of arrival after an initiating event. The classical method for the Rossi experiment used gated circuitry to track when a neutron was incident upon a system. The downside of this method is that the circuitry was complex and only one single fission chain could be measured at once. The modern method allows many chains to be simultaneously measured by a time tagging system such as the LANL custom designed List-mode module (PATRM systems, etc.). The List-mode module allows for custom time binning to take place and the ability to modify the size of the bins post data collection. The experiment is still most accurate near DC, but the List-mode also allows for measurements to be completed in further subcritical regimes. The modern method has many advantages but with those come the disadvantages like the extra analysis step necessary to bin the data and the uncertainty associated with the binning process.

Name: Lillian Miles
Program: UGS
School: Purdue University
Group: XCP-1
Mentor: Abigail Hunter
Category: Engineering
Type: Technical Talk
LA-UR: 14-25923

Modeling Quasielastic Release

A background on material science is given in order to clarify a quasielastic deformation model. Stresses and strains are explained and their relation to plastic and elastic material deformation. Pinned loop and pile-up dislocations are explained along with the Bauschinger effect. Yield surfaces are defined along with isotropic hardening and kinematic hardening and their effect on the yield surface. Deviatoric and volumetric stresses are explained with relation to Hooke's law. The quasielastic model is a shock compression material deformation model run on FLAG. It includes the evolution of deviatoric back stresses caused by the mesoscale effects from pinned and pile-up dislocations as well as stress evolution based on Hooke's law. The quasielastic model includes kinematic hardening and models the immediate reverse plastic flow upon release from shock state. Both theoretical and experimental shock velocity profiles of a quasielastic release are provided.

Name: Joseph Papp
Program: UGS
School: University of Kentucky
Group: MPA-11
Mentor: Rajinder Singh
Category: Engineering
Type: Technical Talk
LA-UR: 14-25525

Gas Transport Characterization of Elastomeric Sealant Materials

Elastomeric materials are commonly used as gaskets, o-rings and adhesives in a wide variety of applications including membrane-based gas separation systems, packaging foams, protective coatings and adhesives. While the mechanical and thermal properties of these seal materials have been analyzed in depth, the gas transport properties are relatively understudied especially at use conditions and configurations. In this study, gas diffusivity and permeability characteristics of common seal materials were determined using a constant volume-variable pressure system. A custom test cell, typically used for gas transport characterization of membrane materials, is used for obtaining He, N2 and CO2 diffusivity and permeability data for fluoroelastomer- and polyurethane- based seal materials as a function of operating conditions. In addition, the influence of cyclic in-situ exposure to elevated temperatures on the gas transport characteristics of these elastomeric seal materials will be presented and discussed. The in-depth gas transport and thermal property characterization studies conducted here for these elastomeric seal materials will provide guidelines for selecting suitable seal material to match membrane gas separation test conditions and will potentially lead to further improvement in the accuracy of the gas transport characterization of membrane materials.

Name: Alicia Swift
Program: GRA
School: University of Tennessee
Group: XCP-3
Mentor: Avneet Sood
Category: Engineering
Type: Technical Talk
LA-UR: 14-25696

Verification of the MCNP6 FMESH Tally

MCNP6 is a Monte Carlo physics code with many capabilities, such as criticality calculations, flux-to-dose conversions, and radiography capabilities. One of the tallies in the code, the FMESH tally, is used to simulate image creation. However, because FMESH tallies do not have some of the same statistical checks as other routines in MCNP6, it is important to conduct verification studies to ensure they are properly representing the physics and statistics of particle interactions. As part of this verification effort, a simple geometry of a monoenergetic (E=10.17 MeV, 5 x 106 simulated particles) neutron pencil beam incident on the center of a graphite slab target was simulated in MCNP6. An ideal detector was placed in the simulation geometry near the slab target on the opposite side of the neutron source. An FMESH tally covered the face of the detector and had time bin widths of 0.5 ns. The time growth of detected particles on the detector screen as simulated by the FMESH tally was then compared with the time growth as estimated by analytic calculations and a similar F4 tally. It was found that FMESH tally results agreed with analytic calculations to within 1.2%, and with F4 tally results to within 4.1%. Therefore, it is believed that, for simple geometries, MCNP6 FMESH tallies represent the physics of neutron scattering very well. Future work should simulate more complicated geometries and cover additional particle reactions.

Name: Jesse Crawford
Program: UGS
School: New Mexico Tech
Group: NIE-IS
Mentor: Giridhar Raichur
Category: Information Technology
Type: Technical Talk
LA-UR: 14-25366

Infrastructure Automation with Puppet

Once IT infrastructure grows beyond just a handful of servers and devices, manual management of devices becomes increasingly impractical. Administering each server by hand often results in inconsistencies that make troubleshooting harder and increase the risk of security exposure due to out-of-date software and noncompliant configurations. This problem has only become more prominent in the modern era of cloud-computing and virtualization where even smaller organizations are managing hundreds of machines.

A new generation of tools for configuration management has become popular over the last few years. One of the most prominent of these "infrastructure automation" systems is Puppet, a powerful open-source server and client that turns "manifests" into direct actions taken to create and configure servers, from operating system to applications. Puppet makes it much easier to manage large IT environments in a way that ensures consistency, visibility, and verifiability of configurations.

Puppet manifests take the form of a lightweight but powerful domain specific language that encourages high-level declarative ("how it should be") rather than imperative ("what puppet should do") manifests, and the puppet ecosystem is enriched by the availability of an enormous number of community-created modules for managing various applications and aspects of operating systems.

Name: Mathew Cherukara
Program: GRA
School: Purdue University
Group: T-1
Mentor: Timothy Germann
Category: Materials Science
Type: Technical Talk
LA-UR: 14-25374

Shock Induced Chemistry in Granular Ni/Al Reactive Intermetallics

Intermolecular reactive composites find diverse applications in defense, microelectronics and medicine, where strong, localized sources of heat are required. However, fundamental questions of the initiation and propagation mechanisms on the nanoscale remain to be addressed, which is a roadblock to their widespread application. The performance and response of these materials is predominantly influenced by their nanostructure, and the complex interplay of mechanical, thermal and chemical processes that occur at very short time scales. Motivated by experimental work which has shown that high-energy ball milling can significantly improve the reactivity as well as the ease of ignition of Ni/Al inter-metallic composites, we present large scale (~41 million atom) molecular dynamics simulations of shock-induced chemistry in granular Ni/Al nano-composites, which are designed to capture the microstructure that is obtained post milling. Shock propagation in these granular composites is observed to be extremely diffuse at low piston velocities, leading to a large inhomogeneity in the local stress states of the material. At higher piston velocities, the shock front is more homogeneous as a consequence of a change in the compaction mechanism; from plastic deformation mediated pore collapse at low piston velocities, to fluid filling of the pores at higher impact velocities. The flow of molten ejecta into the pores subsequently leads to the formation of vortices, where the reaction progresses much faster than in the bulk. While it has been understood for a while now that pores act as initiation sites through the localization of thermal energy, we find that vortex formation in the pores leads to the localization of both thermal and translational kinetic energy, which has consequences both during the initiation process and in the development of the reaction fronts that propagate outwards from the pores. We also follow the evolution of the chemistry to completion after the passage of the shock by allowing the sample to 'cook' under the shock induced pressures and temperatures for up to 0.5 ns. Multiple 'tendril-like' reaction fronts, born in the cauldron of the pores, propagate rapidly through the sample, consuming it within a nanosecond.

Name: Eric Hahn
Program: GRA
School: University of California, San Diego
Group: T-1
Mentor: James Hammerberg
Category: Materials Science
Type: Technical Talk
LA-UR: 14-25670

Physics of High Strain Rate Damage: NEMD Simulation Studies

Studies of spall damage during high strain rate deformation give us insight into the strength and failure of materials under extreme loading conditions. Material strength at high strain rates is a substantial factor in dynamic loading applications ranging from ballistic shielding to inertial confinement fusion. The physics of spallation depends on the complex interplay of material strength, strain rate, shock strength, and potential void nucleation sites determined by microstructure and deformation history. Non-equilibrium molecular dynamics (NEMD) studies allow us to investigate strain rates comparable to those achievable by modern laser and flyer plate shock experiments while providing greater control over shock loading and microstructural variables. NEMD simulations also provide the ability to investigate preferential void nucleation, growth kinetics, and linkage with atomic resolution providing insight into details often indiscernible by conventional experimental methods.

Name: Jonathan Reynolds
Program: GRA
School: Tennessee State University
Group: MPA-11
Mentor: Cortney Kreller
Category: Materials Science
Type: Technical Talk
LA-UR: 14-25488

Characterization of Sensor Response as a Function of Electrode Composition

The Sensors and Electrochemical Devices group at LANL along with Electro-Science Laboratories (ESL) have developed a reproducible mixed potential NOx sensor for application in automotive emission control systems. The pre-commercial sensor has a perovskite working electrode (La1-xSrxCrO3) and a platinum counter electrode, and a YSZ electrolyte layer on one side; with a resistive platinum heater on the other side. While the planar sensor that was developed has been extensively studied, several fundamental questions still need to be answered. This study will attempt to answer the question as to how the performance of the sensor changes as the composition of the working electrode is varied. This study uses a button cell in place of the stick sensor. This cell is constructed using the same materials and processes that formed the stick sensors except that it uses a dense Yttrium Stabilized Zirconium (YSZ) disk with the electrodes on printed on opposite sides. The reason for using the button cell is so that there is a reference electrode, in this case the platinum electrode exposed to a controlled reference gas. With this electrode being an air reference electrode, or an electrode at a known potential due to its environment, the effects of the perovskite working electrode can be isolated and studied. In this study, we will investigate the effects of the changing the Strontium content of the perovskite electrode by using various electrochemical techniques such as Electrochemical impedance spectroscopy (EIS), Cyclic voltammetry (CV), and the voltage response to various analyte gases of interest. The application of these methods to the button cell will allow comparisons of performance with the planar sensors already studied as well as permit predictions as to how the pre-commercial sensor response will change as the compositions in the working electrode is changed.

Name: Anthony Stewart
Program: GRA
School: Southern University & A&M College
Group: NEN-2
Mentor: Tommy Rockward
Category: Materials Science
Type: Technical Talk
LA-UR: 14-25486

Probing the Electrochemical Characteristics of Aged Carbon-Supported Pt Catalysts

In this work we have investigated the effects of aging, by using an Accelerated Stress Test (AST) which consists of voltage cycles from 0.6 V to 1.5 V (V-cycling), on the electrochemically active surface area (EASA) of different types of carbon-supported platinum catalysts. In particular, we employed catalysts supported on two high surface area carbons: XC-72 and graphitized carbon. Both materials are used in the state-of-the-art Proton Exchange Membrane Fuel Cells (PEMFCs). We show a direct correlation between EASA and V-cycling, by utilizing the chemisorption of carbon monoxide and its subsequent oxidation to quantify the active catalyst surface area. These results were obtained by measuring electrochemical characteristics of the catalysts deposited on glassy carbon substrates using various electrochemical techniques such as cyclic voltammetry (CV) and potential step method. Detailed examination of the results has shown that the type of carbon support material plays a critical role in sustaining the catalyst's morphology. This was demonstrated by growth in the so-called double layer region of the CVs, which is indicative of carbon corrosion. In both cases we observed EASA losses as the number of V-cycles increased; however, the rate and extent was higher for XC-72 supported catalyst.

Name: Elizabeth Sooby
Program: GRA
School: Texas A&M University
Group: MST-7
Mentor: Andrew Nelson
Category: Materials Science
Type: Technical Talk
LA-UR: 14-25541

Ion Beam Experiment to Simulate Simultaneous Salt Corrosion and Neutron Damage

A novel technology for Accelerator-based Destruction of Actinides in Molten salt (ADAM) is being developed at Texas A&M University as a method to destroy the transuranics in used nuclear fuel. The core structural components will be exposed to radiation damage by fast-spectrum neutrons and corrosion in 600 °C chloride-based molten salt fuel. An experiment to expose pure nickel, a primary vessel material candidate, to simultaneous molten salt corrosion and ion-beam damage is staged at the Ion Beam Materials Laboratory at Los Alamos National Laboratory. The experiment is designed to allow for a 5.8 MeV, 3 microamp proton beam to pass through the window and deposit approximately 10 displacements per atom (DPA) at the molten salt interface. A surrogate fuel salt, $CeCl_3$-NaCl, is contained in a dry atmosphere capsule held at 550 °C. The first test of this experiment produced a small, pinhole leak in the irradiation sample, therefore ending the experiment early. The initial post-irradiation observations and initial microscopy of the failed sample and experimental assembly are presented here.

Name: Heather Hughes
Program: GRA
School: Arizona State University
Group: IRM-CAS
Mentor: Susan Basquin
Category: Non-Technical
Type: Non-Technical Talk
LA-UR: 14-25049

Sociocultural Dimensions of Literacy/Biliteracy Development

The Laboratory employs many scientists, engineers, and technical workers, as well as graduate students, who bring high levels of education and expertise to the Lab whose first language is not English. These valuable workers are of much importance to the Lab; however, the language barrier causes problems in communicating ideas and results of research and experiments, and also could impair the safety and security within their position. Understanding the linguistic challenges from a sociocultural standpoint is important for the Laboratory because it will ensure higher safety and security overall, along with encourage more effective communication specifically with our foreign nationals. I have worked one-on-one with an English Language Learner (ELL) from Saudi Arabia as a university ELL instructor for two years collecting linguistic data. I stayed in contact with the ELL via e-mail after moving to Los Alamos. My teaching experience, the series of e-mail correspondences, and one full year of graduate-level curriculum development research enabled me to pinpoint certain sociocultural pressures that influenced the literacy/biliteracy development of ELLs. I discovered that these sociocultural pressures also affect foreign nationals at the Laboratory. The accents of foreign nationals/ELLs and the speaking of formal American English to Americans impair the conversational understanding of foreign nationals/ELLs. Conversational misunderstandings prevent the development of relationships and future communications, which in turn causes the foreign nationals/ELLs to become more withdrawn and potentially creating Laboratory hazards. The sociocultural dimensions that foreign nationals/ELLs face are important to the Laboratory and its mission, for all people are our most important resource at the Laboratory, including our foreign nationals.

Name: Nathan L'Esperance
Program: UGS
School: University of New Mexico
Group: IPM
Mentor: Toby Vigil
Category: Information Technology
Type: Non-Technical Talk
LA-UR: 14-25478

ADPSM Document Control and Resumption Process Revisions

The document control and records management (DC/RM) system for ADPSM was staffed by IRM during PF-4 resumption and PF-4 restart. This system has been asked to process a large number of documents and records. This presentation describes the system and the steps taken to optimize efficiency.

Name: Dana Duke
Program: GRA
School: Colorado School of Mines
Group: LANSCE-NS
Mentor: Fredrik Tovesson
Category: Physics
Type: Technical Talk
LA-UR: 14-25405

Studies of Neutron-Induced Fission for 235U, 238U, and 239Pu

The goal of this work is to measure the average total kinetic energy release (TKE) and mass yield distributions in fission at high incident neutron energies. Most of the energy released in fission goes into the kinetic energy of the fission fragments. The TKE and mass information is used to develop fission models which can be used in both energy- and defense-related applications. While the fission process has been studied for decades, little or no data exist for high incident neutron energies for the major actinides. The Los Alamos Neutron Science Center - Weapons Neutron Research (LANSCE-WNR) facility provides a beam of neutrons from 100's of keV to 100's of MeV. A Frisch-gridded ionization chamber is used with thin foil actinide targets to measure the energy and emission angle of the coincident fission fragments. This information is used in the double energy (2E) method to calculate mass yield distributions. Preliminary results for 238U will be presented and the status of the 235U, and 239Pu analyses will be discussed.

Name: Patrick Jaffke
Program: GRA
School: Virginia Tech
Group: T-2
Mentor: Anna Hayes-Sterbenz
Category: Physics
Type: Technical Talk
LA-UR: 14-25108

New Algorithms to Verify Declared Reactor Operations Via Fission Product Isotopics

We present and evaluate computational and analytical solutions for fission product and fissile isotopic abundances in a nuclear reactor and compare these to experimental and other computational sources. Isotopic forensics can provide accurate information on reactor properties, such as the average thermal flux, number of shutdowns, and irradiation time. In particular, we analyze and assign specific long-lived isotopes and their abundance ratios to these reactor history parameters. We determine the effects of altering reactor procedures on the isotopic abundances and also illustrate the importance of nuclear data, such as half-lives, metastable isotope inclusion, and neutron-capture cross-sections, to these calculations by varying nuclear databases.

Name: Mary Kosak
Program: UGS
School: Florida Institute of Technology
Group: XTD-NTA
Mentor: Joyce Guzik
Category: Physics
Type: Technical Talk
LA-UR: 14-25204

Characterizing Amplitude and Frequency Variations in Kepler Pulsating Variables

The Kepler space telescope was launched in 2009 to look for extrasolar planet transits, but Kepler data are also useful for identifying pulsating stars. Pulsating stars are stars that vibrate in different modes and are important for studying stellar interiors and dynamics. We present an analysis of data from the NASA Kepler mission to determine if gamma Doradus and delta Scuti stars have variations in amplitude or frequency of their pulsations. gamma Dor and delta Sct stars are of particular interest because they are slightly more massive (1.5 -2.5 solar masses), hotter (6500 to 8500 K), and larger than the Sun. Through Kepler's Guest Observer program, Dr. Joyce Guzik and Dr. Paul Bradley requested data and classified 2768 potential pulsating star candidates. From this sample, we selected 16 gamma Dor or delta Scuti stars that were observed for 4 or more (80 to 90 day) quarters. The data consist of a photometric data point taken every 30 minutes for each observed star. We performed a wavelet analysis with VSTAR software from the AAVSO (American Association of Variable Star Observers) to see if any of the 16 stars have pulsation frequencies that vary in amplitude. From our results, we determine that the stars' amplitudes do vary from quarter to quarter. In the next phase of this project, we will quantify the properties of the amplitude variations and also search for frequency variations to further characterize the stars. We will also develop and begin to test hypotheses for the causes of the amplitude or frequency variability.

Name: Jeremy Melvin
Program: GRA
School: Stony Brook University
Group: XCP-6
Mentor: Baolian Cheng
Category: Physics
Type: Technical Talk
LA-UR: 14-25609

Evolution of Rayleigh-Taylor Growth After an Initial Richtmyer-Meshkov Instability

We numerically investigate Rayleigh-Taylor (RT) growth on an interface which has an existing Richtmyer-Meshkov (RM) instability already developing. The RM instability is initiated using a variety of shock Mach numbers (Ms = 1.2, 1.5, 2.0, 5.0). After allowing the RM instability to develop for a specified time, a constant gravitational acceleration is applied to the domain, generating a RT growth. We observe the behavior of the mixing fronts and compare them to existing theory for the RT and RM instabilities, developed by Cheng et. al (2002). We observe an insensitivity in the long term asymptotic growth under differing intial shock strengths and an insensitivity to the time at which gravity is initially applied. We find that the existing theory for RM and RT growth matches the growth rates observed in the simulations fairly well.

Name: Taylor Morgan
Program: UGS
School: Brigham Young University
Group: XTD-NTA
Mentor: Joyce Guzik
Category: Physics
Type: Technical Talk
LA-UR: 14-25335

Core Convection, a Driving Mechanism for Gamma Doradus – Delta Scuti Pulsations

Delta Scuti stars lie on the instability strip of the Hertzsprung-Russell diagram where stars undergo self-excited oscillations, pulsating in radial and non-radial acoustic modes with periods of one to several hours. Gamma Doradus stars are nonradial gravity-mode pulsators that lie just at the red edge of the delta Scuti instability strip. They pulsate with periods in the range of 0.3 to 3.0 days. It was originally thought that convective blocking at the bottom of the envelope convection zone was the sole mechanism for driving the g-mode pulsations. However, recent Kepler data shows that stars that are either too hot or too cold for this mechanism to work also exhibit these pulsations. We propose that core convection within gamma Doradus – delta Scuti type stars contributes to driving gravity-mode pulsations. We show results for a 1.62 solar mass model developed to investigate a Kepler gamma Doradus – delta Scuti hybrid, and simulate its core convection using the 3D hydrodynamics code ASH (Anelastic Spherical Harmonic). In order to generate the initial conditions for ASH, we evolve a model using a 1D Lagrangian code MESA (Modules for Experiments in Stellar Astrophysics). The 1.62 solar mass model was initialized with a metallicity of 1.8%, a helium mass fraction of 27%, and a rotation rate of 30% of critical rotation velocity. We also generated theoretical 1.85 and 2 solar mass models to study their core convection. The spherical ASH simulations use 100 radial points, 256 latitudinal points and 512 azimuthal points, which is sufficient to include stellar convective cores less than 1e10 cm in diameter. Our 1.62 solar mass model was run in ASH for over 600,000 timesteps, or a period of about 3.5 years, to allow the development of convective mixing.

Name: Brandon Runnels
Program: GRA
School: California Institute of Technology
Group: T-3
Mentor: Irene Beyerlein
Category: Physics
Type: Technical Talk
LA-UR: 14-24380

A New Model for Interface Energy

Understanding interfacial energy between crystal lattices is of great interest in modeling mechanical behavior of multiphase materials and in understanding and predicting interface stability in the context of multi-material laminate composite design. However, due to the exceedingly complex nature of most interfaces, it is difficult to analyze interfaces in the general case. A semi-analyical model is proposed here that attempts to approximate interface energy for the general case, and to find the locations of sharp local minima in the energy landscape ("energy cusps") exactly. It is hypothesized that the coherence (i.e. matched crystal periodicity) across an interface is the dominant effect in interfacial energy. Based on this assumption, an interface energy model is formulated. It is then tested with symmetric tilt boundaries in FCC and BCC materials, as well as for bicrystal orientations such as Kurdjumov-Sachs. Reasonable agreement with data gathered from molecular dynamics simulations is observed, implying that the original hypotheses are valid.

Name: Daniel Shields
Program: GRA
School: Colorado School of Mines
Group: LANSE-NS
Mentor: Fredrik Tovesson
Category: Physics
Type: Technical Talk
LA-UR: 14-24875

SPIDER Progress Towards High Resolution Correlated Fission Product Data

The SPIDER detector (SPectrometer for Ion DEtermination in fission Research) is under development with the goal of obtaining high-resolution, high-efficiency, correlated fission product data needed for many applications including the modeling of next generation nuclear reactors, stockpile stewardship, and the fundamental understanding of the fission process. SPIDER simultaneously measures velocity and energy of both fission products to calculate fission product yields (FPYs), neutron multiplicity (ν), and total kinetic energy (TKE). A detailed description of the prototype SPIDER detector components will be presented. Characterization measurements with alpha and spontaneous fission sources will also be discussed.

Name: Mitchell Wood
Program: GRA
School: Purdue University
Group: T-1
Mentor: Marc Cawkwell
Category: Physics
Type: Technical Talk
LA-UR: 14-25575

Molecular Dynamics Simulations of Chemistry Induced by Void Collapse in RDX

Chemical reactions in solid explosives under impact begin at ‘hot spots’ triggered by collapsing voids where the local temperature can exceed by several thousands of degrees above those in the bulk. Pore collapse and the leading chemical events occur on extremely short timescales (a few 10’s of picoseconds and up) and within regions of a few nanometers, making their direct experimental observation challenging. However, these length and time scales are ideal for molecular dynamics (MD) simulations. We show with multi-million atom reactive MD simulations and evolution of hot spots during void collapse in single crystals of the explosive molecular crystal RDX. For a fixed impact velocity we have found that the diameter of the void controls the formation of the ejecta and subsequent energy localization. Sweeping through void sizes in the range of 10 to 40nm, we find that the critical pore diameter for self-sustained chemistry to be 40nm for a 2km/s impact. Aspects of non-equilibrium chemistry are discussed within our simulations through careful analysis of the molecular species, their populations, in addition to the vibrational and center of mass temperatures. Over many simulations, we have found that the amount of RDX decomposition is commensurate with the pore size but that the exothermic chemistry required to sustain or grow a hot-spot is not. Growth and quench rates of the sustained reaction front have been measured and provide key insight into the first steps of the shock to deflagration transition in molecular explosives.