Los Alamos National Laboratory

“Celebrating Student Achievement”

16th Annual Student Symposium Abstracts

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UNM-LA
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It is estimated that two billion people, about a third of the human population, are infected with Tuberculosis (TB), with 9 million deaths worldwide. Early detection and diagnosis of TB can potentially reduce associated morbidity and mortality. A significant challenge is the ineffectiveness of the current diagnosis, and the lack of a “gold standard”. Current diagnostics such as sputum cultures, blood cultures, and urine lipoarabinomannan (LAM) assays tend to have low sensitivity, which varies with HIV co-infection, the age of the patient, and other environmental factors. Our team has developed a novel approach called lipoprotein capture to measure LAM in patient blood, and are currently in a clinical trial in Uganda to evaluate the diagnostic. To overcome the limitations of data analysis, we implemented a statistical model that combines the test results of sputum cultures, blood cultures, urine LAM assays with data from our lipoprotein capture assay. The statistical model uses Bayesian data augmentation to calculate the posterior probability that each individual is TB positive given the data. The model is flexible in that we can select specificity and sensitivity of the various diagnostics, include local propensity of TB adjusted for HIV status, age and other covariates. We use Monte-Carlo Markov chain to calculate the distribution of individual probability of being TB positive, and show how these predictive distributions can be used to identify the most relevant subset of tests to perform to best predict TB status. The outcome of the analysis and the efficacy of our Lipoprotein capture method in diagnosing active TB in patients will be presented.
Evaluation of Water Soluble Sacrificial Layers to Fabricate Thin and Elastic PU

Thin and flexible Polyurethane (PU) membranes have significant potential for organ-on-a-chip applications. However, PU can stick to the substrate on which it is spin cast, making it quite difficult to effectively remove and use such membranes. The objective of this project is to investigate different materials as water soluble sacrificial layers on which the PU can be coated. The sacrificial layer should dissolve in water allowing for the PU to be lifted off. We are investigating three potential candidates for the sacrificial layer, which include: Poly Vinyl Alcohol (PVA), Dextran, and Poly Acrylic Acid (PAA). A solution of each material is spin coated on the substrate and dried to obtain a thin film coating. The substrate is then spin-coated with PU. The PU is then cured and the substrate is submerged in water to release the PU film. Different parameters such as the thickness of the sacrificial layer, water temperature, dissolution time, and sonication can impact the ability to reproducibly lift off the PU film. In this work, we will identify the optimal approach to release the PU membranes. The membranes will then be used to fabricate an organ on a chip platform (e.g. Heart or Lung) and to demonstrate a biophysical function (e.g. pumping or breathing).
The alveoli in the human lung contain specific cell types, namely Alveolar Type I (ATI) and Alveolar Type II (ATII) cells. To recapitulate this cellular microenvironment in a tissue engineered lung, it is important to have the ability to co-culture the two types of cells and maintain their ratio similar to that found in the human lung (roughly 95% ATI cells). However, these cells have been shown to transdifferentiate, as well as dedifferentiate into mesenchymal-like cells in an in vitro culture condition. The motivation behind this study was to identify a cell source and culturing environment for alveolar lung cells (ATI/ATII) cells that can maintain human like cellular micro-environment in vitro. In this work, we investigated the ability of primary human small airway epithelial cells (SAEC) as the cell source for our artificial lung. We attempted to replicate previous experiments where SAEC cells were cultured and a mixed population was achieved, but we subjected the cells to differing types of culturing environments in respect to relative stiffness. Traditionally, cells are grown on polystyrene plates; however, it was our interest to additionally investigate the effect of trans-well plates and polyurethane (PU) membranes to obtain the desired ATI/ATII cell ratio. Each of these substrates possesses unique stiffness and allow for investigation of the influences of air/liquid interface. In addition, the PU membranes can be subjected to cyclic stress similar to regular breathing patterns. Cells were microscopically imaged and RT-PCR was performed for confirmation of a mixed ATI/ATII cell population. At the end of this project, we expect to identify a suitable cell source for the downstream devices and an optimized protocol for cell culture on variable surfaces. This work will greatly facilitate the development of miniaturized tissue-engineered artificial lungs to act as an in vitro model for drug toxicity studies.
Rational Protein Design for pH Switchable Antibody Purification Tool

The ability to modulate antigen-antibody interaction is key to the development of novel therapeutics, affinity chromatography reagents and diagnostic tools. The binding of protein G with the Fc region of human immunoglobulin G (antibody) is useful in antibody isolation and purification. Protein modeling drove the structure based mutagenesis carried out on protein G to include three amino acid substitutions to change the functionality of the protein by adding polar and charged amino acids. The Protein-protein interaction interface of the previously mutated binding region of Protein G was again modified via direct amino acid mutagenesis to replace an asparagine on the periphery of the binding site with glutamic acid or aspartic acid. Changing the pH in the presence of this new polar amino acid was expected to cause it to be protonated (positively charged) or deprotonated (neutral). The change in polarity in the outskirts of the binding region would cause a differential binding with the target Fc region of human immunoglobulin G (antibody), making this a pH “switchable” interaction. The project helps gain understanding in protein-protein interaction and improve the level of expertise in Molecular Biology and protein engineering.
RNA viruses cause many significant diseases worldwide, such as Dengue and Yellow fevers, the Flu, AIDS, etc. These viruses evolve very rapidly and few antiviral therapeutics and vaccines exist to treat them. The exact mechanism for viral evolution remains poorly understood.

We are studying the evolution of RNA viruses using an in-vitro / laboratory environment. 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. Although we are currently focused on the human Influenza-A (IAV) virus, we hope our model can be applied to other RNA based viruses. 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 to express proteins that the IAV naturally produces (supplemental cells). After a series of infections within the supplemented cell lines, we will study the effect of this supplementation on the viral evolution. We expect that the viral population will evolve to efficiently infect the supplemental cells and lose the ability to infect the wild type (natural) cells. If our hypothesis is correct, this approach may provide novel viral therapeutic approaches.
Almost one-third of the world’s population is infected with latent tuberculosis (TB). About 10% of those infected have a potential risk to develop active TB at some point in their life. The current gold standard for diagnosis of TB are time consuming and laboratory intensive, while other methodologies are insensitive, and have poor specificity as well. The problem is even more severe in pediatric populations, as children are unable to cough out sputum, making the diagnosis more challenging. A simple blood-based test would alleviate this problem, and could potentially be extended to extra-pulmonary TB as well, and this is the goal of our work. To detect presence of tuberculosis biomarker lipoarabinomannan (LAM) in blood, we have developed a modified sandwich assay (exploiting reliable antibodies supplied by FIND) to capture LAM in human serum, which is carried by high-density lipoprotein molecules in blood. Our fieldable assays are deployed using a waveguide-based biosensor platform developed at Los Alamos National Laboratory. We demonstrate, for the first time, detection of LAM in human serum of adult and pediatric population with active TB along with other co-morbidities. As observed in some of the test assays, the assay might work not only as diagnostic, but also as prognostic. The diagnostic is in process of validation in two heavily disease-burdened populations in Kenya (pediatric) and Uganda (adult), results from both are provided. Analysis and interpretation of the data is challenging because of the use of multiple corroborative gold-standards, each of which has its own limitations. To overcome this, a Bayesian model has been developed to interrogate the results of our diagnostic trial (Wall, and Bridgewater poster). Herein, our novel lipoprotein capture approach and the results of the validation studies will be presented.
How Ionizing Radiation Affects the Human Cells – The Basics

Most people fear ionizing radiation. Certainly it can cause death if we are exposed to too much, and the most recent symbol for it makes it clear to stay away from it. Why is ionizing radiation dangerous? When atoms in living cells become ionized one of three things usually happen – the cell dies, the cell repairs itself, or the cell mutates incorrectly and can become cancerous. Not all cells are affected by ionizing radiation in the same way. The cells that reproduce the most and are the least specialized are the most likely to be affected by ionizing radiation, for example those in a forming fetus. Radiation-induced ionizations may act directly on the cellular component molecules or indirectly on water molecules, causing water-derived radicals. Radicals react with nearby molecules in a very short time, resulting in breakage of chemical bonds or oxidation (addition of oxygen atoms) of the affected molecules. The major effect in cells is DNA breaks. DNA double-strand breaks induced by ionizing radiation are considered the most relevant lesion for mutation and carcinogenesis. Radiation induced bystander effect (RIBE) was found in 1990 and challenged the conventional dogma that no effects were expected in cells that had not been exposed to radiation. We studied the mechanisms underlying RIBE, which enlightened us on directions to radiation protection against low-dose environment radiation as well as during radiotherapy.
Surrogate MDR Evolution: Bacillus Anthracis Sterne and Yersinia Pestis A1122

To mitigate the potential threat of multidrug resistance (MDR) in pathogens as biological warfare agents (BWAs), we must generate non-pathogenic MDR surrogates and understand the genomic evolution towards MDR. The dramatic increase in the number of bacterial pathogens acquiring antimicrobial resistance (AMR) and MDR poses a threat to our nation’s health and security, especially when they are intentionally used as BWAs. Bacillus anthracis (causative agent of anthrax) and Yersinia pestis (causative agent of the plague) are two such potential BWAs. In September 2001, the “Amerithrax” terrorist attack utilized refined spores of B. anthracis targeting media institutions and government officials, resulting in 22 confirmed cases of anthrax and increased awareness of BWAs. Y. pestis, responsible for the death of half of Europe’s population during The Black Death, could be an aerosolized BWA. Clearly, the acquisition of AMR/MDR, through natural or artificial means, to these and other pathogens will greatly reduce the efficacy of our already diminished array of antimicrobial treatments. Surrogates permit safe testing of various novel candidate drugs without the need for highly regulated and costly Select Agent and/or BSL-3 facilities. Understanding the genomic evolution towards AMR/MDR by sequencing the associated mutations will also offer significant insight into the mechanisms of AMR/MDR. To generate safe MDR surrogates, we evolved B. anthracis Sterne and Y. pestis A1122, KIM6, and KIM10 to be resistant to various antibiotics. Bacteria were subjected to selective pressures on plates containing 3× the minimum inhibitory concentration of specific antibiotics. Resistant mutants were isolated and used for subsequent selection rounds on other antibiotics. To verify the presence and evolution of genes conferring resistance, the AMR/MDR surrogate isolates will be sequenced and compared to the sequence of the parent strain. The generated AMR/MDR strains will form a validated panel that can be used in reference laboratories to test new therapeutics.
Shamia Pamplin, (NEN-2); Yulin Shou, (B-10); Armand Dichosa, (B-10); Elizabeth Hong- Geller, (B-DO); Patrick Chain, (B-10); Kumkum Ganguly, (B-10) Los Alamos National Laboratory, Los Alamos, NM 87545 The City of Albuquerque Environmental Health Department, the New Mexico Department of Health and the Bernalillo County Health Protection Section announced in July, 2016 that 2 cases of human tularemia, also known as rabbit fever, have been confirmed from Bernalillo County. Francisella tularensis is the etiological agent of tularemia, a serious and occasionally fatal disease of humans and animals. F. tularensis is a common gram negative bacterium that is found throughout the United States, but is most commonly located in the central states e.g., Missouri, Arkansas, Illinois, Oklahoma, Tennesee. F. tularensis is transferred to humans from tick bites, deerflies, and undercooked meat. This bacterium can live for long periods in cold, moist environments and can be used as a bio threat agent. We are studying the growth pattern, morphology and antibiotic susceptibility of F. tularensis vaccine strain LVS and developing the surrogates, which are resistant to Ciprofloxacin and Doxycycline, the most commonly used antibiotics against tularemia. These surrogates will facilitate the drug development and screening against pathogenic F. tularensis.

**An Overview of The Disease Tularemia Caused by Francisella tularensis**

Shamia Pamplin, (NEN-2); Yulin Shou, (B-10); Armand Dichosa, (B-10); Elizabeth Hong- Geller, (B-DO); Patrick Chain, (B-10); Kumkum Ganguly, (B-10) Los Alamos National Laboratory, Los Alamos, NM 87545 The City of Albuquerque Environmental Health Department, the New Mexico Department of Health and the Bernalillo County Health Protection Section announced in July, 2016 that 2 cases of human tularemia, also known as rabbit fever, have been confirmed from Bernalillo County. Francisella tularensis is the etiological agent of tularemia, a serious and occasionally fatal disease of humans and animals. F. tularensis is a common gram negative bacterium that is found throughout the United States, but is most commonly located in the central states e.g., Missouri, Arkansas, Illinois, Oklahoma, Tennesee. F. tularensis is transferred to humans from tick bites, deerflies, and undercooked meat. This bacterium can live for long periods in cold, moist environments and can be used as a bio threat agent. We are studying the growth pattern, morphology and antibiotic susceptibility of F. tularensis vaccine strain LVS and developing the surrogates, which are resistant to Ciprofloxacin and Doxycycline, the most commonly used antibiotics against tularemia. These surrogates will facilitate the drug development and screening against pathogenic F. tularensis.
Identification and Selection of Growth-Promoting Bacteria in C. Sorokiniana 1412

A growing body of literature indicates that many microalgae, including biofuel production strains, require bacteria to provide essential nutrients and metabolites for optimal growth and survival. Nevertheless, most of the research conducted to improve the productivity of commercial algal systems relies on extrapolating growth studies conducted under axenic laboratory conditions, despite the fact that many algal production systems contain hundreds to thousands of species of bacteria. By traditional cultivation standards, it is not possible to recapitulate and assess even 1% of the possible intercellular interactions that positively (or negatively) influence algal productivity during cultivation. To address this need, we integrated gel microdroplet (GMD) technology with microfluidics to generate millions of culture microdroplets (MDs), whereby sequestering unique cell-to-cell interactions to facilitate both rapid identification and recovery of growth promoting bacteria via flow cytometry. Herein, we describe both the pipeline using off-the-shelf, commercially available technologies and the process by which microbial candidates that increase algal production are selected.
The growing need for alternative fuel sources through the use of cellulosic (non-food) biomass is becoming increasingly important to today’s society. Lignin, water insoluble dry plant matter, contains up to 25% of the total weight of non-food biomass; however, there is not an efficient process to readily convert lignin into bio-fuels. An easier conversion of lignin to useable biofuels could potentially replace up to 30% of the U.S. petroleum consumption. Recent research developed an extractive ammonia pretreatment that solubilizes Lignin and facilitates its catalytic degradation. Nature’s solution to breaking down lignin into viable products is lignin peroxidase (LiP), an oxidative enzyme. The goal of this project was to engineer a LiP with enhanced catalytic properties and jump start the biomass to biofuel conversion process. LiP activity depends on formation of a catalytic oxygen radical by a surface exposed tryptophan (Trp171) residue aid by a heme group. We are engineering LiP by substituting the catalytic tryptophan residue for a more polarizable synthetic amino acid, selenatryptophan (Se-Trp). By replacing this catalytic residue with a heavy-metal tryptophan analog, the redox potential of the enzyme should therefore increase, enhancing lignin degradation. The use of pretreated soluble lignin and improved LiP presents a highly efficient route for lignin valorization and ultimately bio-fuel commercialization. Progress towards the biotransformation of our Se-containing tryptophan analogs using tryptophan synthase and their subsequent bio-incorporation into LiP are presented.
Pre-Determined Protein Assembly of sfGFP into Nanofibers for Biosensing Applications

Protein assemblies offer precise, novel molecular structures with functional diversity. However, assembling functional proteins with pre-defined structures presents a key challenge. Green fluorescent protein (GFP) originates from a species of jellyfish, and is an important biological marker for protein expression. Pre-determined assembly of GFP may report even minimal levels of target protein activity. To do this, we attempted to assemble a version of a fluorescent protein that lights up upon formation of long fibrils. Earlier work by a LANL team successfully split an eleven-stranded superfolder GFP (sfGFP) into 10+1 strands, 9+2 strands or 9+1+1 strands, which combine to form a fluorescing protein made of two linked GFPs (a dimer). Our work focuses on the creation of two ‘dark’ constructs from the sfGFP full-length sequence. On their own, these constructs contain a missing strand; but, when simultaneously present in a cell, they combine in a chain of potentially infinite length and fluoresce. We engineered this behavior by creating a gene library of 10^10 combinations of construct 1 and construct 2. We co-expressed the constructs under an IPTG inducible promoter in bacterial cells. Upon induction, we observed varying fluorescence under the illuminator. Upon analysis on a flow cytometer, we observed a wide distribution of fluorescence intensity in the cell population, with at least two resolvable peaks. We selected the brightest cells through fluorescence activated cell sorting (FACS). The sorted population was regrown and confirmed to fluoresce. Preliminary efforts at protein isolation through native PAGE (polyacrylamide gel electrophoresis) show that the constructs combine to make a tetramer, although we suspect the constructs should create an even longer fiber. Next steps include more attempts at protein isolation, as well as DNA sequencing of the strong variants, electron microscopy to verify construct assembly, and size exclusion chromatography experiments.
Defining a Protocol for Neuromuscular Junction Formation Using C2C12 and NSC-34 Cells

Neuromuscular junction (NMJs) are the connection between muscles and neurons that drive muscle contractions. NMJs grown in vitro can be used to test a variety of pharmaceuticals and countermeasures that are meant to alleviate the effects of diseases and toxins that affect their function, e.g. ALS and sarin gas. NMJs, however, are difficult to grow and there is no set protocol as to assure consistent formation of NMJs. There has been progress using supplements in media that gear differentiation of myoblasts and neuronal cells through the use of chemical signaling that parallels embryogenesis. One such supplement is retinoic acid (RA) which is said to regulate insulin-like growth factor (IGF) a growth hormone which is seen to promote myoblast differentiation and has neurotrophic qualities. Horse serum (HS), which is used in C2C12 myoblast differentiation, is also said to regulate the expression of IGF. Using RA, IGF, and HS in different combinations for the differentiation of C2C12 and NSC-34 cell lines, we report a co-culture protocol that helps foster the formation of NMJs.
Validation of an Improved Lipid Inducible Fluorescent Algal Bioswitch

Lipid producing microalgae used for biofuels are of significant interest because they can be used as an alternative energy source to fossil fuels. Using microalgae for biofuels has many advantages including their compatibility of their product with existing engines and because they absorb carbon dioxide as they grow. Microalgae based biofuels are also favorable because they do not require agricultural land to grown on and can be grown in waste water. The availability of microalgae biofuels for commercial use is extensively impeded by the high costs of growing, harvesting and processing lipid producing algae. The high costs emerge from specialized instrumentation and time required to grow and harvest algae. We have created a bioswitch, a sensor-regulator system, which senses high concentrations of lipids within the algae and expresses a green fluorescent protein in response. Specifically, the unicellular microalgae, STA6-Chlamydomonas reinhardtii (Cr), was a model organism to test our bioswitch. Our bioswitch uses a lipid sensing transcription regulator (FadR) to control the expression of a fluorescent protein marker (GFP) and is cloned into the Cr’s chloroplast, the site of lipid production. Fluorimeters will be used to identify the optimal stage of lipid production for harvesting. A Fluorimeter is a very low-cost instrument, which will replace the need for expensive instruments and can be easily deployed to the production fields. By creating and validating this bioswitch, we would reduce the need and cost for expensive instruments, thus aiding algae biofuels to become more accessible for commercial use.
It is estimated that two billion people, about a third of the human population, are infected with Tuberculosis (TB), with 9 million deaths worldwide. Early detection and diagnosis of TB can potentially reduce associated morbidity and mortality. A significant challenge is the ineffectiveness of the current diagnosis, and the lack of a “gold standard”. Current diagnostics such as sputum cultures, blood cultures, and urine lipoarabinomannan (LAM) assays tend to have low sensitivity, which varies with HIV co-infection, the age of the patient, and other environmental factors. Our team has developed a novel approach called lipoprotein capture to measure LAM in patient blood, and are currently in a clinical trial in Uganda to evaluate the diagnostic. To overcome the limitations of data analysis, we implemented a statistical model that combines the test results of sputum cultures, blood cultures, urine LAM assays with data from our lipoprotein capture assay. The statistical model uses Bayesian data augmentation to calculate the posterior probability that each individual is TB positive given the data. The model is flexible in that we can select specificity and sensitivity of the various diagnostics, include local propensity of TB adjusted for HIV status, age and other covariates. We use Monte-Carlo Markov chain to calculate the distribution of individual probability of being TB positive, and show how these predictive distributions can be used to identify the most relevant subset of tests to perform to best predict TB status. The outcome of the analysis and the efficacy of our Lipoprotein capture method in diagnosing active TB in patients will be presented.
Data-driven Modeling of Gram-negative Multi-drug Resistant Tripartite Efflux Pumps

The increasingly prevalent phenomenon of antibiotic resistance in Gram-negative bacteria calls for a comprehensive analysis of the mechanisms through which pathogens extrude toxic substrates from within cells into the external environment. Resistance-Nodulation-Division (RND) pumps, a family of multi-drug resistant (MDR) efflux pumps, are one such mechanism, catalyzing the active efflux of many antibiotics and chemotherapeutic agents by forming tripartite complexes with outer membrane channels and periplasmic adaptor proteins. In this study, we use a fully automated and data-driven modeling pipeline (implemented as a web server) developed in our group to produce and investigate various atomic models. The web server first builds homology models of the individual pump components based on a library of experimental crystal structures. The final tripartite models are constructed from these components via a series of structural alignments and targeted geometric simulations to published cryo-EM structures. Here, we build and examine six Escherichia coli RND pumps (AcrAB-TolC, AcrAD-TolC, AcrEF-TolC, EmrAB-TolC, YhiUV-TolC), eleven Pseudomonas aeruginosa RND pumps (AdeABC, MexAB-OprM, MexCD-OprJ, MexEF-OprN, MexHI-OpmD, MexJK-OprM, MexPQ-OpmE, MexVW-OprM, MexXY-OprM, MuxABC-OpmB, TriABC-OpmH), and five Burkholderia RND pumps across four separate species (CeoAB-OpcM, AmrAB-OprA, AmrAB-OprM, BpeAB-OprB, BpeEF-OprC) with the goals of defining the physicochemical properties that enable uptake of various compounds into bacterial cells and of developing more effective pharmaceutical techniques to circumvent drug resistance.
Assessing and Tuning Ruthenium Catalysts for Self-Healing Applications

Ruthenium catalysts have been shown to be efficient for ring-opening metathesis polymerization, a powerful method for forming materials with wide biomedical, self-healing, and engineering applications. Extensive modifications of the ligand system have led to dramatic advances in initiation and propagation rates of the polymerization reaction and catalyst stability. However, we envisioned a catalyst for self-healing materials with a fast initiation rate, a modest propagation rate to widen the scope of viable monomers, and high catalyst stability in solution to maintain self-healing functionality. This work aimed to screen various commercially available ruthenium catalysts for such properties via UV-Vis spectroscopy and 1H-NMR with procedures widely used since their publication in 2001 by the Grubbs lab. Catalyst decomposition rate in solution was also analyzed using 1H-NMR. In addition, modifications to the catalyst ligand system were made in an effort to tune catalyst stability and its kinetic properties.
From the 1940’s to the early 2000’s, Pajarito Canyon was home to a series of experiments known as the critical experiments. These experiments, numbering over 50,000, provided valuable information about various isotopes of uranium and plutonium such as their critical masses, cross sections, and general behavior. While the critical assembly program is no longer in existence at the Pajarito site, the data is still studied and employed in various fields of nuclear research. At the present time, three of the critical assemblies, Comet, Flattop, and Godiva, have found a new home at the Nevada Test Site where additional measurements will be obtained. A general survey of each of the major assemblies is presented in an effort to illuminate the significance of the work done at the Pajarito Site and demonstrate an evolution in the understanding and applications of nuclear criticality.
Separation of Fast Neutron Activated Titanium for Post-Detonation Nuclear Forensics

In nuclear forensics, nuclear or radiological materials are characterized by their physical, chemical, isotopic, microstructural, and morphological properties. The information determined through such characterization of materials then allows for government and law enforcement agencies to correctly trace the origin of nuclear or radiological materials either seized or dispersed into the environment. In this work extraction chromatography will be employed to isolate small amounts of scandium (46Sc, 47Sc, and 48Sc) produced from activated titanium (46Ti, 47Ti, 48Ti, 49Ti, and 50Ti) to enable determination of n-p cross section values. Batch studies were performed using Eichrom's Ln and DGA resins in hydrochloric and nitric acid matrices to separate trivalent scandium from tetravalent titanium. Separation factors of 102 and 105 were measured using LN and DGA resin and are calculated from the k’ or retention factor of the analytes to the resin. Adaption of the batch study to a wet slurry column allowed for separation of Sc from Ti at milligram quantities. A column elution profile was determined and the separation will be scaled up to gram quantities. The scale-up will be performed using larger columns and higher loading capacities. Elution fractions were analyzed using Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES).
The purpose of the Chemistry and Metallurgy Research Replacement (CMRR) Project is to ensure the continuation of analytical chemistry (AC) and materials characterization (MC) capabilities at Los Alamos National Laboratory (LANL) for the National Nuclear Security Administration’s (NNSA’s) mission and programs. One of the essential functions of the CMRR Project is to transition AC and MC operations from the Chemistry and Metallurgy Research (CMR) building to the Radiological Laboratory/Utility/Office Building (RLUOB) and Plutonium Facility-4 (PF-4). Transferring AC/MC capabilities from CMR to RLUOB and PF-4 requires rigorous planning, preparation, and execution of the operational start-up requirements to demonstrate the readiness of laboratory infrastructure, procedures, and personnel training. This capability transfer is being conducted by the CMRR Transition to Operations (TTO) team. This poster will describe the overall CMRR project and the various tactics used by the CMRR TTO team for preparing the start-up of operations in accordance with the TA-55 New Activity Approval Process. The immediate goal of the CMRR TTO team is to plan and execute operational start-up planning and preparation, management self-assessments, and equipment testing and method validation in support of the 2019 Program Milestone (termination of programmatic operations in the CMR facility). The planning process requires the determination of the logistics to determine the logistics of operations by preparing process flow diagrams, determining the required materials and standards for operations, and transferring the existing process-specific procedures at CMR to TA-55. All these tasks are essential for the successful facility transfer and maintenance of AC and MC capabilities for NNSA missions at LANL.
Morphological Analysis for Materials Attribution (MAMA) for Analysis of Morphology

Forensic analysis of special nuclear materials (SNM) samples provides valuable information on material compositions, histories, etc., and may be further augmented by identification of morphological signatures obtained through optical or electron microscopy. The MAMA (Morphological Analysis for Materials Attribution) software package provides tools designed specifically for the quantification of SNM morphological signatures for this purpose. Users are able to identify, distinguish, and quantify particles or sets of particles in microscopy images using the MAMA software. The segmentation feature of the software allows users to select from preset equations and to adjust the parameters of the equations to automatically apply particle-particle and particle-background division. After applying the best fit segmentation, users may then manually adjust segment lines to more accurately fit the image, as well as distinguish between different particle types and the background. The software also offers quantification of parameters to describe the particles and/or particle subsets in the sample, i.e., vector area, equivalent circular diameter, and circular area. Exporting the raw data allows for further analysis of the data and provides the capability to compare data sets and delineate defining parameters of specific SNM samples. The distinction of these parameters may provide the ability to distinguish SNM samples of different origins by their discrete morphological signatures.
First Row Transition Metal Adsorption on Actinide Resin

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 is a unique environmental sample formed under extreme conditions and 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 such as extraction chromatography in order to isolate, characterize, and determine the nuclear material within the debris. Matrix constituents, including the first row transition metals, could inhibit these radioanalytical techniques and subsequent determination by ICP-AES. The research focuses on further characterizing Actinide Resin for the first row transition metals that could be found within post-detonation debris or could interfere with ICP-AES analysis. No research has been published on the adsorption of most of first row transition metals on Actinide Resin. Actinide resin is an extraction chromatographic resin that is commercially available from Eichrom Technologies, LLC. The resin is based upon the extractant bis(2-ethylhexyl)methanedisphosphonic acid (H2DEH[MDP] or "DIPEX®"), which is supported on the inert polymeric substrate Amberchrom CG-71ms acrylic resin beads. Actinide resin displays extremely high extraction coefficients for metals with oxidation states +3 and above. Batch contact experiments were conducted in order to determine the retention capability of Actinide Resin for the first row transition metals. The eluate collected from the conclusion of each transition metal batch contact experiment was analyzed on a Thermo Scientific iCAP 7000 Series ICP-OES.

2016 Annual Student Symposium
Unnatural heavy metal-containing amino acid analogs have shown to be very important in the analysis of protein structure, using methods such as X-ray crystallography, mass spectroscopy, and NMR spectroscopy. Synthesis and incorporation of selenium-containing methionine analogs has already been shown in the literature however with some drawbacks due to toxicity to host organisms. Thus synthesis of heavy metal tryptophan analogs should prove to be more effective since the amino acid tryptophan is naturally less abundant in many proteins. For example, bio-incorporation of β-seleno[3,2-b]pyrrolyl-L-alanine ([4,5]SeTrp) and β-selenolo[2,3-b]pyrrolyl-L-alanine ([6,7]SeTrp) has been shown in the following proteins without structural or catalytic perturbations: human annexin V, barstar, and dihydrofolate reductase. The reported synthesis of these Se-containing analogs is currently not efficient for commercial purposes. Thus a more efficient, concise, high-yield synthesis of selenotryptophan, as well as the corresponding, tellurotryptophan, will be necessary for wide spread use of these unnatural amino acid analogs. This research will highlight our progress towards a synthetic route of both [6,7]SeTrp and [6,7]TeTrp, which ultimately will be used to study the effect on the catalytic activity of Lignin Peroxidase (LiP).
As the world struggles to satisfy the ever increasing demand for clean energy, one of the most promising sources of clean electricity is hydrogen fuel cells. The major challenge associated with current hydrogen technology is the safe storage of hydrogen due to its inherent physical properties. A solution is the chemical storage of hydrogen in stable molecules that can be induced to release hydrogen gas in the presence of a catalytic species on demand. Amine boranes are considered one of the most attractive classes of compounds for hydrogen storage due to their high hydrogen density and tendency to readily dehydrogenate under mild conditions. In this project, a series of thorium and uranium metal complexes: bis(pentamethylcyclopentadienyl) complexes (C5Me5)2An(NMe2)2 (An = Th, (1), U (2)) and tris(hexamethyldisilyl)uranium species U[N(SiMe3)2]3 (3) were synthesized in order to investigate the compounds’ reactivity towards amine boranes (R'R"NHBH3 (R = R" = Me; R = tBu, R" = H; R = R" = H). Preliminary results show complexes 1 and 2 readily dehydrogenate amine boranes at RT in 2 h at 2 mol % catalyst loading. Vigorous gas evolution is observed and the conversion to dehydrogenated products is quantified by 1H and 11B NMR spectroscopy. Initial stoichiometric results suggest NMe2 transfer to the amine borane, eliminating R2N–BH–NMe2. Upon heating, precatalysts 1 and 2 undergo cyclometallation and elimination of HNMe2 to afford metallaaaziridines 1a and 2a as described in the literature for group 4 complexes. Further exploration into catalyst activation and the catalytic activity of complexes 1-3 is ongoing.
Mo-99 (66 h half-life) decays to Tc-99m, the dominant medical isotope used in nuclear medicine. The Office of Material Management and Minimization (M3) within the National Nuclear Security Administration (NNSA) has an objective to ‘accelerate the establishment of a reliable, commercial Mo-99 supply network that avoids a single point of failure and does not use proliferation-sensitive HEU (High Enriched Uranium)’. This remit includes a cooperative agreement with SHINE medical technologies, a company aiming to produce Mo-99 domestically in the US. SHINE plans to use a deuterium-tritium neutron generator to produce fission Mo-99 from Low Enriched Uranium (LEU) sulfate solutions. Therefore, the determination of uranium concentration in uranium sulfate solutions is an important consideration for SHINE. Utilizing the Beer-Lambert Law allows for uranium concentration analysis using the characteristic visible absorption spectra of the uranyl cation dissolved in 1 mol/L sulfuric acid. The molar absorptivity (ε) at λmax was calculated previously using accurate standard solutions, with different UV-vis cells tested, impurities screened and data collection methods refined. However, comparison with the Davis-Gray uranium analysis technique revealed the importance of temperature control for accurate and precise measurement, with ε varying significantly as a function of temperature. To address this issue a newly installed Peltier unit was used to control cell temperature and ε determined from freshly prepared standard solutions over a range of uranium concentrations at a fixed temperature. To test the accuracy and precision of the refined technique, the concentration of uranium of 10 unknown samples were then measured at the same temperature. Finally, the impact of temperature on ε was analyzed for uranium, not just in 1 mol/L sulfuric acid but also 1 mol/L nitric and hydrochloric acids, thus facilitating an evaluation of technique general applicability.
A Lexicon for Consistant Description of Morphological Features in Nuclear SEM Images

This lexicon was developed in order to provide a consistent form of labeling morphological features seen in scanning electron microscopy (SEM) images. The lexicon is accompanied by a flow sheet that shows a step by step process of how the lexicon works, as well as a definitions of the terminology, in order to provide a ubiquitous analysis through all users. Here, we provide examples to show how the lexicon can be used to characterize surface textures and features, as well as particle size, structure, and distribution. The lexicon can be used as a standalone product, but it also has been incorporated into the MAMA software for use with labeling and categorization of images within the program.
The water-gas shift (WGS) and reverse water-gas shift (RWGS) reactions play important roles in ammonia, hydrocarbon, methanol, and hydrogen manufacturing, as well as in the development of alternative fuels production. These reactions require a heterogeneous catalyst or a Lewis acidic homogeneous catalyst. Lanthanides are good Lewis acids and may be capable of catalyzing the WGS and RWGS reactions. A redox active cerium metal center paired with sterically demanding spectator ligands is a viable candidate for such a catalyst. Through breaking the reaction mechanism into a series of homogeneous intermediates, the reaction can be conducted stepwise by generating the requisite cerium complexes.
One of most important ongoing questions in molecular actinide chemistry is to what extent 5f and 6d orbitals participation in covalent bonding. Understanding this phenomenon, which has remained unresolved for decades, would contribute significantly to a better understanding in bonding across the actinide series; such knowledge can facilitate advancement of chemical separation technologies in treatment of used nuclear fuel. My group at Purdue University has contributed, in part, to answering this long-standing question by synthesizing and studying a uranium tris(imido) moiety. We took this approach since subtle electronic effects and contrasts in bonding among metals becomes more apparent when considering the existence of multiply bonded species. Though this study was important for understanding bonding in uranium complexes, it shed no light on bonding trends across the actinide series. In fact, a large majority of actinide chemistry involves the study of uranium, leaving most of the transuranic elements relatively unexplored. Los Alamos National Laboratory (LANL) is one of the few places that has the availability and knowledge to safely work with transuranic elements. At LANL I am attempting to translate the methodology used for the synthesis of a uranium tris(imido) to make the analogous neptunium and plutonium complexes to allow elucidation of bonding across the actinide series.

**Understanding Bonding in the Actinides: Synthesis of Np and Pu Tris(imido) Complexes**

One of most important ongoing questions in molecular actinide chemistry is to what extent 5f and 6d orbitals participation in covalent bonding. Understanding this phenomenon, which has remained unresolved for decades, would contribute significantly to a better understanding in bonding across the actinide series; such knowledge can facilitate advancement of chemical separation technologies in treatment of used nuclear fuel. My group at Purdue University has contributed, in part, to answering this long-standing question by synthesizing and studying a uranium tris(imido) moiety. We took this approach since subtle electronic effects and contrasts in bonding among metals becomes more apparent when considering the existence of multiply bonded species. Though this study was important for understanding bonding in uranium complexes, it shed no light on bonding trends across the actinide series. In fact, a large majority of actinide chemistry involves the study of uranium, leaving most of the transuranic elements relatively unexplored. Los Alamos National Laboratory (LANL) is one of the few places that has the availability and knowledge to safely work with transuranic elements. At LANL I am attempting to translate the methodology used for the synthesis of a uranium tris(imido) to make the analogous neptunium and plutonium complexes to allow elucidation of bonding across the actinide series.
Domestically produced ethanol is an important component of gasoline; however, the use of ethanol is capped at ten percent. New techniques to efficiently convert lignocellulosic biomass to ethanol have surfaced, giving rise to a massive supply of ethanol. In order to take advantage of this cheap, renewable feedstock as well as preserve national energy security, it has never been clearer that a method for upgrading ethanol to fit current infrastructure needs to be developed. In order to be cost competitive with petroleum products, our method needs to find pathways for making both fuels and relevant fine chemical precursors to offset production costs. We have examined the self-condensation of acetaldehyde, which can be obtained from ethanol via dehydrogenation. We have demonstrated production of long chain even numbered aldehydes, importantly 2-ethylhexanal, directly from acetaldehyde. 2-Ethylhexanal, along with other aldehydes, was synthesized under mild conditions and can be used as an important and diverse chemical precursor for surfactants, fuel additives, cosmetics, plasticizers, etc. The reactions can also be performed in ethanol and water, providing a pathway to create potential fuels and additives while making the process potentially solvent-waste free. This methodology shows the potential to provide a range of fuels and industrially necessary chemical feedstocks that fit within the current energy infrastructure, and with further refinement, this process can be a potential long term and stable solution to a growing foreign oil dependency problem.
Nuclear fission produces multiple lanthanide isotopes, many of which yield valuable insights into the type and origin of nuclear material. The ability to carefully separate and analyze selected lanthanide radioisotopes can be a key tool for nuclear forensic applications. However, adjacent lanthanides are notoriously difficult to separate from each other due to their very similar chemistry. One effective method for separation of lanthanide cations is High Performance Liquid Chromatography (HPLC). HPLC techniques have long been used to separate lanthanides, and our goal is to modernize our current capabilities through the development of a new test system. The chemistry is well developed, selective stripping of trivalent lanthanide cations from a cation exchange resin using α-hydroxyisobutyric acid (HIBA), but instrumentation advances yield scope for process improvements. Recently, a new HPLC system has been installed comprising of quaternary pumps, columns, fraction collectors and a Diode Array detector that allows for post column on-line analysis. Addition of PAR (4-(Pyridylazo) resorcinol)) for post column derivatization facilitates accurate determination of lanthanide cation elution using the diode array detector. The yellow to red color change upon lanthanide complexation is monitored through absorbance at both 414 and 530 nm. Initial work focused on determination, and then removal, of resin impurities that interfered with colorimetric detection. Single lanthanide cations were then run through the HPLC to ‘map’ the system before moving to more complex mixtures. Finally, the impact of variations in HIBA concentrations and solution pH has been studied for a lanthanide separation of relevance to nuclear forensic applications, the separation of Eu, Sm, Tb and Y. Eu and Sm are adjacent lanthanide elements while Y behaves like a lanthanide element adjacent to Tb.
Nuclear Forensic Signatures Using Destructive and Non-Destructive Methods

Nuclear forensic investigations can benefit from the application of both non-destructive assay (NDA) and destructive assay (DA) methodologies. While NDA methodologies typically cannot provide the same level of precision as DA methodologies, they can typically provide results in a timelier manner and without impacting the integrity of the sample. The timely results from NDA methodologies can assist in the performance of DA methodologies by providing an initial estimate of analyte concentration so that the optimum internal standard quantity and/or analytical dilution factors can be decided in advance. NDA results can also guide decisions on which DA methodologies may best meet the objectives of a nuclear forensic investigation. This poster will report on our efforts to improve the uncertainty estimate of a NDA methodology that uses high-purity germanium (HPGe) detectors and FRAM software used to analyze the resulting spectra. This NDA methodology can provide valuable information on the isotopic enrichment of plutonium or uranium materials. However, it is important that the uncertainty of the reported plutonium or uranium enrichment not be underestimated, as otherwise incorrect conclusions may be reached. This poster will also report on our effort to provide an improved radiochemical DA method for the quantifying Am-241 in weapons grade plutonium (WGPu). Americium-241 is an important chronometry indicator given its in-growth from the Pu-241 isotope present in WGPu. Minimizing the uncertainty of the Am-241 concentration in WGPu can be of value in determining the chronometry of a plutonium material.
Distributed Memory Implementation of Coupled Cluster

In this work we explore performance and parallelization strategies for Coupled Cluster, a method for approximately solving properties of quantum many-body systems. By exploiting symmetries of the physical system, efficient implementations of Coupled Cluster involve the creation, storage, and multiplication of large block-diagonal matrices. Here we present strategies to distribute and balance computation over many nodes, to reduce communication requirements, and to improve cache performance. Our goal is indefinite weak scaling with respect to an increased number of particles and model accuracy.
Programming an Adiabatic Quantum Computer

Since the unveiling of D-Wave’s 16-bit adiabatic quantum computer, the company has scaled all the way up to a 1,152 qubit computer called the D-Wave 2x -- with feasible plans to reach 10,000+ qubits in the next five years. The technology is finally beginning to become viable to solve some interesting problems, and adiabatic quantum computing is starting to be a compelling avenue for reaching faster computing speeds. As the D-Wave computer scales to larger and more applicable capabilities, the methods for programming it need to be improved upon. Currently, there are several software packages that D-Wave has released that are useful for mapping certain types of problems. While these are helpful, there is still much work to do: programming the quantum computer is still by no means an easy thing to do. To an extent, you currently have understand how the qubits are interacting in order to use it. This would be the equivalent of knowing what’s going on with the bits when programming to a classical computer. In this poster, I first discuss the current state of adiabatic quantum computing and how the D-Wave 2x works. I then go through some simple examples of programming to the D-Wave 2x, to show how difficult it currently is to solve simple problems. After discussing some of the programming problems, I present my research into solving some of these, as well as future work that will attempt to abstract these hardware details from the user. The ultimate goal is for the quantum programmer to not have to know anything about the qubits themselves. This will allow users to focus on solving their problems rather than thinking about the underlying hardware.
Virtual Reality: The Future of Visualization?

When the phrase virtual reality (VR) is thought of within the context of popular culture, it may conjure up images of movies like The Matrix for some, or of the holodeck in the Star Trek universe for others. While those capabilities do not yet exist, the current generation of VR tech is a far cry from the older generations, which range from room-filling and budget-draining cave automatic virtual environment (CAVE) setups to large, heavy, claustrophobic VR helmets. This summer we worked with the HTC Vive to test the capabilities and limitations of said device in a bid to see how VR head-mounted displays (HMDs) can be applied to lab science, specifically in the area of scientific data analysis and visualization.
Resilient Off-Grid Microgrids: Capacity Planning and N-1 Security

Over the past century, the electric power industry has evolved to support the delivery of power over long distances in highly interconnected transmission systems that span large geographic regions. Despite this evolution, in some parts of the United States and other parts of the world, some communities are not connected to these systems. These communities rely on small, disconnected distribution systems, i.e., microgrids to deliver power. More importantly, perhaps, there is a general trend to support microgrid development within large transmission systems for economic, environmental, and reliability reasons. However, microgrids are not held to the same reliability standards as transmission grids and can place many communities at risk for extended black-outs. To address this issue, we develop an optimization model and algorithm for capacity planning and operations of microgrids that includes N-1 security and other modeling features. The effectiveness of the approach is demonstrated using the IEEE 13 node test feeder and a model of the Nome, Alaska distribution system.
**Performance Studies of Parallel Erasure Coding on Clustered Micro Storage Servers**

This project covers the benchmarking for a cluster of micro storage servers that are used for encoding files and then distributing them, this is called erasure coding. MPICH (a Message Passing Interface) will be used in tandem with ZFEC (an open-source erasure coding library) in order to test the speeds of encoding the files in parallel. For a baseline, drives were initially tested in isolation for encoding speeds that can then be compared to the speeds of the encoding done in parallel. There are two generations of micro storage servers, each with its own advantages, these comparisons will help better understand which advantages are worth having/cost effective.
Exploring Performance of Domain Decomposition Strategies for MC Radiation Transport

SuperNu is a Monte Carlo (MC) radiation transport code to simulate light curves of explosive outflows from supernovae. The MC transport step is domain replicated. To enable scaling on next-generation HPC systems, we implemented the recursive coordinate bisection approach of domain decomposition for the opacity calculation. Then, we propagated the decomposition to other steps in the simulation and constructed a communication infrastructure to support the decomposition. In this poster we demonstrate the results of two communication schemes: the Improved KULL and Improved Milagro algorithms. We present results from a range of processors: Ivybridge, Haswell on local clusters at LANL and the AMD Bulldozer Opteron 6200 series processors at Blue Waters’ Cray XE6 nodes. Finally, we tested the scalability of SuperNu on the latest Intel Xeon Phi architecture, Knights Landing.
Swarm Optimization for Parameter Calibration of the SURF Reactive Burn Model

The particle swarm optimization (PSO) method and its variant the fully informed particle swarm (FIPS) method are well-established metaheuristics for searching multidimensional parameter spaces characterized by multiple local minima. Both methods are characterized by swarms consisting of N particles of dimension d represented as pseudo vectors containing parameter values. Each particle has a fitness value f, determined by the problem of interest. Particle positions are iteratively updated in parameter space through a comparison with the swarm’s fitness (FIPS) or with a combination of social and cognitive fitness (PSO). The swarm continues to update until either a fitness or iteration threshold is met. Although the common approach to parameter calibration for reactive burn models is user trial and error, PSO has proven effective for reactive burn model calibration (Handley et al., 2015). This work will discuss the implementation of both the PSO and FIPS methods for calibration of the SURF reactive burn model to velocity gauge data obtained from gas gun experiments for the high explosive PBX 9502 (95% Triaminotrinitrino benzene, 5% Kel-f by mass). 1D FLAG Hydrocode simulations were conducted from within the PSO/FIPS codes. The accuracy of each method was first determined using synthetically created velocity gauge data. SURF parameter values were then obtained during calibrations to both single shot and multiple shot constraining data sets. Finally the accuracy of the resulting parameters was evaluated using experimental data not included in the calibration.
A Web Developer's Toolbox

Author: Jade Comellas, University: University of New Mexico, Group: DCS-ISS, Mentors: Sandy Frost and Ron Crotzer, Title: A Web Developer’s Toolbox

The internet is used by more than 40% of the world’s population, yet very few people know anything about how web pages work. Most people accept it as magic or fail to even wonder what is going on in the back end when they submit their information through an online form or use a web page to access information imported from a database. The “magic” behind a web page can be thought of as a series tools in a toolbox. These would include SQL, Python, HTML, CSS and JavaScript. With knowledge of these programming languages and how to use them together, anyone could create a good looking, interactive and informative webpage, which is a very important and helpful skill in today’s world with the increasingly high demand for web development. Each of the previously mentioned tools play their own important role in creating a web page. Based on simple experiments, a spreadsheet filled with data can be imported into a database and then added to a website using Python to conduct the process, SQL to manage the database, and HTML to create the structure of the web page. CSS and JavaScript can then be used to make it attractive and interactive. Having a full toolbox is a powerful way to solve a vast number of problems. Since many people have the need for their work, forms or spreadsheets to be published on the web, the combined use of SQL, Python, HTML, JavaScript and CSS is continuing to become more powerful. For example, the form used to register for the student symposium could easily be converted into a web page using these basic programming tools. There are endless ways to use this skill, including ones that had once nearly seemed to be impossible for many people.
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**Development of a Web Interface for Search and Visualization of Self-DescribingDataSet**

Data analysis can be a tedious job if not given tools that help search and visualize the data. Echo software is an implementation of a data analysis tool, but to be able to use it you need programming background in order to search the data, plot it and analyze it. With this project we look forward into expanding echo software capabilities in a webpage that includes features for searching and plotting in a user-friendly manner and reduce the time it takes to find relevant data. In our implementation of the website we developed a faceted and full text search to apply filters, query a database and receive amount of data files based on searched or selected parameters. After applying filters the user is given the option to plot the data files with interaction capabilities, save the image or download into analysis software.
Virtual Reality: The Future of Visualization?

When the phrase virtual reality (VR) is thought of within the context of popular culture, it may conjure up images of movies like The Matrix for some, or of the holodeck in the Star Trek universe for others. While those capabilities do not yet exist, the current generation of VR tech is a far cry from the older generations, which range from room-filling and budget-draining cave automatic virtual environment (CAVE) setups to large, heavy, claustrophobic VR helmets. This summer we worked with the HTC Vive to test the capabilities and limitations of said device in a bid to see how VR head-mounted displays (HMDs) can be applied to lab science, specifically in the area of scientific data analysis and visualization.
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The Darwin cluster in the Advanced Co-design Laboratory is an advanced research and development test bed. It contains a diverse set of computers with cutting edge and unique architectures networked together to form a heterogeneous HPC system. This cluster supports our multidisciplinary co-design projects by providing a space where code can be run on a variety of different hardware layouts. The users of Darwin need proper tools and data about the machines to be able to effectively make use of it. Developers need to have access to readily available and updated benchmarking information to help them optimize their programs for new and complex hardware configurations, and find the best tool for the job. There is also interest in granting access to students, new staff, and visitors to have the opportunity to explore and understand what the machine is and what is inside. Getting a tour of the server room is access controlled, and although you might physically see the nodes, it is generally an uninformative experience. Our goal is to create an interface that allows all types of users to explore the contents of the cluster through an easy to use touchscreen display. Bringing together a benchmark management system, an inventory management system, and the resource management information available through SLURM, we intend to make available as much information about the cluster as possible through the use of large-format touchscreen displays, a GUI/web tool, and benchmark reports for the hardware in the Darwin cluster.

**User-friendly Exploration of a Heterogeneous Cluster**

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We demonstrate performance metrics of an Object Oriented Fortran code with GPU acceleration enabled through NVIDIA/PGI’s CUDA and OpenACC on different GPU architectures. We also examine using multiple OpenMP threads to allow GPU porting with codes that natively contain OpenMP and Fortran. PGI’s support of OO-Fortran enables a wider range of scientific problems to be accessible on fewer resources by leveraging the power of a graphics card. As an example, spectral element methods have been shown to be arithmetically intensive, suggesting significant speedup can result from parallelization on GPUs. An open source OO-Fortran spectral element library, SELF, is parallelized using OpenACC and OpenMP. Code performance is examined using a Tesla M2090 (Fermi microarchitecture) and Tesla K20 and Tesla K40 (Kepler microarchitecture) with the cuBLAS library and different code restructuring to play to the strengths of GPUs.
Particle Swarm Optimization Parameter Study

The problems of science and engineering require the location of global minima within high-dimensional, multi-modal search spaces. Particle swarm optimization is a gradient-free algorithm that is useful for traversing these search spaces. The behavior of a particle swarm is dependent on three parameters: inertial, cognitive, and social. Previous work has provided guidance for a choice of parameters that result in a stably performing algorithm. In addition to this work, we examined the effects of particle swarm size in relation to dimensionality. In this poster, we compared the particle swarm algorithm’s performance with a dynamically updated inertial weight parameter to the linearly updated and fixed inertial weight parameters. Additionally, we tested the performance of the algorithm with a variation of fixed particle swarm sizes, inertial weights, cognitive and social parameters. Through this series of tests, we have developed guidelines for the choice of particle swarm parameters such that the algorithm will have a greater probability of converging to the global minima in high-dimensional, multi-modal search spaces.
Malicious computer software, commonly known as malware, is an increasing problem for the US government. Malware written by advanced persistent threat (APT) actors is a dire threat both to the security of our critical infrastructure systems and to the integrity of our intellectual property. When a new piece of malware is created, existing defenses often fail to detect the threat, and thus do not prevent the harm the software will cause. Security analysts constantly analyze emerging malware and accordingly augment their organization’s defenses to stop malware. Current analysis methods are from two distinct perspectives: one globally looks at a set of huge known software with machine learning approaches to classify the software as benign or malicious, and the other closely examines malware samples one by one. When the macro analysis view fails, analysts must resort to the micro analysis view. The micro view usually forces analysts to start over from scratch for each sample. Our aim is to improve the analysts’ productivity by combining the best characteristics of the micro and macro analysis views to form a new mid range view. To do this, we offer collaboration and a deep malware similarity analysis, integrated with one of the most widely used reverse engineering tools in the industry, IDA Pro. There are existing IDA Pro plugins that offer collaborative features and malware similarity scoring. However, all existing approaches are stuck in the micro view of analyzing only one or two malware samples at a time. Our approach allows for the malware analyst to compare their current sample to many already analyzed samples in our database and retrieve anything that is similar. The purpose of this is to effectively share previously done work, avoiding the start from scratch situation. Not only does it give the analyst means to collaborate and have a good starting point, our approach allows for the analyst to save and share their work for future use.
SuperNu is a Monte Carlo (MC) radiation transport code to simulate light curves of explosive outflows from supernovae. The MC transport step is domain replicated. To enable scaling on next-generation HPC systems, we implemented the recursive coordinate bisection approach of domain decomposition for the opacity calculation. Then, we propagated the decomposition to other steps in the simulation and constructed a communication infrastructure to support the decomposition. In this poster we demonstrate the results of two communication schemes: the Improved KULL and Improved Milagro algorithms. We present results from a range of processors: Ivybridge, Haswell on local clusters at LANL and the AMD Bulldozer Opteron 6200 series processors at Blue Waters’ Cray XE6 nodes. Finally, we tested the scalability of SuperNu on the latest Intel Xeon Phi architecture, Knights Landing.
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Interoperability Across GPU Languages and Platforms

As researchers look towards exascale computing for large scientific applications, the portability and composability of GPU parallelism becomes a vital endeavor. CUDA and OpenCL are specialized, low-level programming of GPU hardware, while OpenACC and OpenMP4 are higher-level languages tailored for portability, as details are left to the compiler. How these methodologies perform together is the focus of this research. We assess current interoperability and the performance of a large-scale grid running the Game of Life on GPUs.
Optimization of Interatomic Potentials using Machine Learning

Molecular dynamics simulations are an indispensable tool in chemistry, biology, and materials science for studying the dynamical evolution of a system in atomistic detail. The simulations require an interatomic potential as a physical basis from which the forces acting on the atoms are computed. The interatomic potentials used most commonly in molecular dynamics simulations are composed of simplified functional forms that require parameterization. The quality and physical accuracy of interatomic potentials depends sensitively on the quality of the parameterization. However, the parameterization of interatomic potentials is normally difficult and for complex models with many parameters it cannot be done by hand. We have created a new, efficient, and general optimization package “EPO” (Empirical Potential Optimizer) that automatically refines a parameterization to quantify and minimize errors with respect to a database of high quality reference data. Utilizing a number of different machine learning techniques, EPO may be used for any system for which parameterizations are non-optimal. The application of EPO to the generation of new parameterizations for the LANL-developed quantum molecular dynamics code LATTE will be presented.
In this work we explore performance and parallelization strategies for Coupled Cluster, a method for approximately solving properties of quantum many-body systems. By exploiting symmetries of the physical system, efficient implementations of Coupled Cluster involve the creation, storage, and multiplication of large block-diagonal matrices. Here we present strategies to distribute and balance computation over many nodes, to reduce communication requirements, and to improve cache performance. Our goal is indefinite weak scaling with respect to an increased number of particles and model accuracy.
Between the 1970s and 1990s, Los Alamos National Laboratory built and utilized a largely custom computer network for the Lab’s supercomputers. Designed to support the unusual performance, storage, and security requirements of an American weapons lab, the Los Alamos Integrated Computer Network, as the focus of historical study, complicates and enriches the history of computer networking development, exploring the approaches and contributions to computer networking of an institution outside the better-known worlds of industry, academia, and the military. For example, the Lab’s reticence to adopt TCP/IP due to performance and security concerns further complicates the narrative of the ARPANET/Internet protocol suite’s adoption among advanced networking sites in the 1980s and 90s.

The Route Less Taken: The Homegrown Los Alamos Integrated Computer Network
Distributed Memory Implementation of Coupled Cluster

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**Optimal Transmission Line Switching under Geomagnetic Disturbances**

In recent years, there has been an increasing concern about how Geomagnetic Disturbances (GMDs) impact a reliable operation of electrical power grids. Of particular interest are the Geomagnetically-Induced Current (GIC) flows that can saturate transformers, resulting in hotspot heating and increased reactive power losses. Such negative effects can potentially cause catastrophic damage on transformers and severely impact the ability of a power system to reliably deliver power. Hence, we develop a model of transformer heating as a function of the regular Alternating Current (AC) and GIC, also integrate increased reactive power load into power flow equations. In this paper, we solve an optimization problem of minimizing the total generator dispatch cost and load shedding cost subject to AC power flow constraints and transformer heating constraints with an option of switching transmission lines. We employ state-of-the-art convex relaxations of nonlinear AC power flow equations and disjunctive bilinear relaxations to obtain tight lower bounds on the objective. We demonstrate on a modified IEEE RTS96 system (single area) that such a model is computationally tractable and the option of line switching is effective to mitigate the effects of GIC on the grid. We also provide a sensitivity analysis of operating decisions with respect to the directions of GMDs.
Deep Convolutional Neural Networks for Image Tagging

Image tagging, which involves generating a list of objects that are present in an image, represents a critical technology for automated image search. Convolutional neural networks have exceeded human performance on a popular whole image labeling task, which require the algorithm to generate a single label for each image. However, good performance on whole image labeling depends on the image to contain a single object, a condition that is often violated in image tagging tasks. Much work has been focused on the more difficult problem of object detection, which requires the algorithm to draw a tight bounding box around every instance of every target object, a task that currently requires complex algorithms and expensive computations to achieve state-of-the-art results. Here, we show that we achieve comparable results with a simpler model. We train our model using 16X16 labeled image patches, with each patch containing instances of objects drawn from 20 target categories. We then aggregated the heat maps for each target category into a list of tags in images from the VOC 2007 detection task. Our preliminary results show an improvement image tagging results versus an approach based solely on whole image classifications, and comparable results versus state-of-the-art detection tasks reduced to image tagging.
Guiding Performance Optimization using the Roofline Model on Proxy Applications

The performance of different proxy applications relative to the performance of the hardware has become important to exploiting the full capabilities of next generation systems. Benchmarking different proxy applications is becoming more important to understand where there is opportunity to improve performance. The way you benchmark a proxy application is through calculating the Arithmetic Intensity. One of the new ways to map out the performance space for hardware is using the Roofline Model. This project is calculating the Arithmetic Intensity of CLAMR, PENNANT, NuT, SNAP and then plot these on the Roofline Model.
Analysis of Trinity Power Metrics for Automated Monitoring

Trinity’s size has caused a need for alternative methods of system monitoring. Current methods involve the use of humans, system administrators, to visually detect anomalies. However, with the significant increase in node counts on Trinity, these methods are impractical. Applying machine learning techniques to data to detect anomalies enables the system administrators to concentrate on solving problems. This work utilizes Intel’s Data Analytics Accelerated Library (DAAL) to implement machine-learning techniques for analysis of Cray power metrics. A k-means clustering algorithm is applied to the data set as a means to “cluster” data from similar performing nodes. While most nodes have similar hardware not all will have similar workloads. For example, we can expect to see power consumption of an active node to be different than that of an idle node. Similar performance differences can be observed between applications of different intensities; i.e. an application that is compute intensive vs. data intensive. This clustering leads us towards a power consumption baseline for the system. After an adequate number of clusters have been determined, Principal Component Analysis (PCA) is used to measure the variance within a cluster and as a way to compare baseline vs. runtime performance. By applying these algorithms we can determine anomalous events and through further analysis establish when and where events occurred. This methodology will be used in future work on other Trinity monitoring data sets to determine system wide event correlations.
Discrete Event Simulation of Nuclear Waste Production and Storage

In addition to legacy waste already stored at LANL, programs essential to the mission of Los Alamos produce transuranic (TRU) waste. For safety and legal reasons, only a limited amount of TRU waste can be stored on site. With the TRU waste outlet, WIPP, not currently accepting waste, LANL is in a position of uncertainty as to when they will be able to dispose of their TRU waste. This is of concern because if TRU waste storage reaches full capacity, all research and production which generates TRU waste will be significantly hampered. The two main limitations of storage are the number of drums of material and material at risk (MAR). Variables that affect the amount of drums and MAR that can be stored include multi-stacking, container types, damage ratios, waste type, and the availability of storage areas. In order to demonstrate the usefulness of discrete-event simulation modeling to aid in the assessment of TRU waste storage capacity relative to waste generation schedules, a model was created and exercised using notional input data with those variables as input parameters. With the model, a user can easily change these input parameter variables to evaluate how long—and at what magnitude—operations can be sustained while staying within TRU waste storage limits.
User-friendly Exploration of a Heterogeneous Cluster

The Darwin cluster in the Advanced Co-design Laboratory is an advanced research and development test bed. It contains a diverse set of computers with cutting edge and unique architectures networked together to form a heterogeneous HPC system. This cluster supports our multidisciplinary co-design projects by providing a space where code can be run on a variety of different hardware layouts. The users of Darwin need proper tools and data about the machines to be able to effectively make use of it. Developers need to have access to readily available and updated benchmarking information to help them optimize their programs for new and complex hardware configurations, and find the best tool for the job. There is also interest in granting access to students, new staff, and visitors to have the opportunity to explore and understand what the machine is and what is inside. Getting a tour of the server room is access controlled, and although you might physically see the nodes, it is generally an uninformative experience. Our goal is to create an interface that allows all types of users to explore the contents of the cluster through an easy to use touchscreen display. Bringing together a benchmark management system, an inventory management system, and the resource management information available through SLURM, we intend to make available as much information about the cluster as possible through the use of large-format touchscreen displays, a GUI/web tool, and benchmark reports for the hardware in the Darwin cluster.
An Automatically Parallelizing Compiler for a Pure Functional Language

In the world of high performance parallel computing, imperative programming languages suffer from the consequences of unrestricted mutable state: Race conditions are practically unavoidable, requiring delicate synchronization, and increasingly frequent hardware faults necessitates proportionately more frequent whole-program checkpointing to have any expectation of successful termination. Our project promises an alternative. Pure functional languages have no concept of variable assignment, only definition. With the guarantee against side-effects, data dependencies are transparent and independent expressions can be programatically identified and safely evaluated in parallel. Similarly, because of this referential transparency, any unit of computation that fails due to hardware fault needs only its inputs to be restarted (rather than the whole state of the program). Our work thus far includes a serial implementation of an intermediate representation of Haskell -- known as STG -- used by the Glasgow Haskell Compiler (GHC) and a test suite of more than 1400 test cases. As a convenience for testing, we have also extended this language to something more expressive; a proper subset of Haskell. We are currently developing the parallel runtime and working on using the interface provided by GHC as a front-end to target full Haskell source code and translate their representation to ours.
Metadata Indexing Service System-Reengineering, Enhancement, & Generalization

The primary goal of Parallel Metadata Indexing Service System (PMIS) is to provide consistent and secured metadata indexing service to clusters with various file systems, such as LANL's new MarFS storage ecosystem. PMIS collects metadata from file systems and inserts the data into the MongoDB server. Indexing data via MongoDB allows users to quickly and efficiently query the metadata that contains information about the file. In this project, we reengineered and enhanced SearchTool, a previously built PMIS. SearchTool was originally built with MongoDB 2.0 and Pymongo 2.2, and has not been enhanced since then. It is critical for SearchTool to adapt to the latest development environment not only to eliminate the security blind spots, but also improve performance. Therefore, the primary goal of this project was to rebuild SearchTool with current versions of the previously mentioned software. In addition, I focused on making it easier to set up configuration files and provided updated documentation so that developers and users can easily use and interpret this system. Moreover, by implementing polymorphism I simplified the complicated structure of the original program. As a result, initial processing time was significantly reduced while maintaining quality and functionality of the system. Finally, I present an empirical analysis including performance comparison in different sharding environments and validate our implementation’s ability to query large scale metadata indexes. In the future, we plan on developing user-friendly applications for the system and addressing possible security leaks.
The Effect of Polymorphism of CEMs on Their OPA and TPA Properties

Conjugated Energetic Molecules (CEMs) are known to have photon absorption property of carbon based conjugated molecules and high nitrogen content of high explosives (HEs) which makes them ideal for direct optical initiation of photo active HEs. Furthermore, their one-photon absorption (OPA) and two-photon absorption (TPA) occur at optical ranges that could be excited by conventional laser. These optical properties unlike in molecular CEMs, could be influenced by polymorphism in the crystalline CEMs. Polymorphism is a structural variation in crystalline forms of molecules which can be due to crystal packing, existence of different conformers or hydration of the crystals. In this study, time-dependent density functional theory (TD-DFT) was used to investigate the effects of polymorphism on OPA and TPA properties of crystalline CEMs and the fundamental role of intermolecular couplings on nonlinear optical processes.
Virtualization has become the tool used by cloud providers and data centers to achieve high utilization of their computing resources based on demand. It is not a tool widely used in HPC applications because of its implicit performance overhead. However, recent new container virtualization implementations such as Docker sees near-native performance and could be a solution for improving HPC utilization of resources. We perform an extensive performance evaluation of container based Docker and traditional Infrastructure as a Service (IaaS) virtualizations for CPU, Memory, I/O and Network resources using industry-standardized benchmarks like SpecCPU, Linpack, Netperf, IOZone, RAMspeed SMP, and STREAM. Future work would measure the isolation performance of KVM, Xen, Docker and LXC.
Here at Los Alamos National Laboratory we have many important projects going on at all times. The only problem is that we have yet to establish a collaboration tool that can assist us in communicating with other organizations as we carry out these important tasks. Our solution to this problem was to research a variety of Open Source Social Software’s that may be useful to our cause here at the laboratory. This software package will build more connections making it easier to share information. We carried out this research by comparing a variety of Open Source Social Software’s to a Gartner Evaluation Criteria Excel Sheet which we modified to see which software meets our specific needs best. Based on our findings we picked a couple of software packages that we believed would be good contenders in our research. We then installed them to get a more descriptive look at what abilities they had. In this process we gain skills in computers, knowledge on software, and experience in research. We also learned that communication is vital for growth in the work that the laboratory does. The more connected the laboratory is the better it can work as a team to accomplish its mission.
Adaptive Graph Partitioning Methods for Quantum Molecular Dynamics

A novel graph-based electronic structure theory has recently been developed. This graph-based approach is used to optimize the density matrix build in quantum-based molecular dynamics (QMD) simulations based on the recursive second-order spectral projection (SP2) method. It combines the advantages of a tunable thresholded sparse matrix algebra with the natural parallelism of a divide and conquer approach. This makes it ideal for applications to the next generation exascale computing in the near future. Most advanced algorithms in QMD simulations are evaluations of matrix polynomials. In order to efficiently parallelize these evaluations at each time step, it has been shown that one can formulate a data dependency graph, G_i, that is estimated from the density matrix at the previous QMD time step. The vertex set of G_i is then partitioned with a specially defined objective function in order to determine how to compute the polynomial evaluations in parallel. Previous approaches have used tools like METIS followed by simulated annealing to improve the objective value. It is however expensive to use these methods to solve a new graph partitioning problem at each time step. In this work, we show that it is sufficient to refine the solution of the previous time step based on the current graph instead of solving a new graph partitioning problem. We also propose a modified version of the current simulated annealing algorithm and another inspired by Kernighan-Lin as refinement methods. To support our claim and demonstrate our refinement methods, we analyze several systems that exhibit different chemical connectivities and report the difference between refining a previous partitioning versus creating a new one.
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Collaborative IDA Malware Analysis Plugin (CIMAP)

Malicious computer software, commonly known as malware, is an increasing problem for the US government. Malware written by advanced persistent threat (APT) actors is a dire threat both to the security of our critical infrastructure systems and to the integrity of our intellectual property. When a new piece of malware is created, existing defenses often fail to detect the threat, and thus do not prevent the harm the software will cause. Security analysts constantly analyze emerging malware and accordingly augment their organization’s defenses to stop malware. Current analysis methods are from two distinct perspectives: one globally looks at a set of huge known software with machine learning approaches to classify the software as benign or malicious, and the other closely examines malware samples one by one. When the macro analysis view fails, analysts must resort to the micro analysis view. The micro view usually forces analysts to start over from scratch for each sample. Our aim is to improve the analysts’ productivity by combining the best characteristics of the micro and macro analysis views to form a new mid range view. To do this, we offer collaboration and a deep malware similarity analysis, integrated with one of the most widely used reverse engineering tools in the industry, IDA Pro. There are existing IDA Pro plugins that offer collaborative features and malware similarity scoring. However, all existing approaches are stuck in the micro view of analyzing only one or two malware samples at a time. Our approach allows for the malware analyst to compare their current sample to many already analyzed samples in our data base and retrieve anything that is similar. The purpose of this is to effectively share previously done work, avoiding the start from scratch situation. Not only does it give the analyst means to collaborate and have a good starting point, our approach allows for the analyst to save and share their work for future use.
OpenMP is a programming model to increase on node parallelism in applications. It often comes under attack for poor performance compared to MPI everywhere. This is because OpenMP is conventionally used at the loop level and thus suffers from high thread start up costs and thread synchronizations. A higher-level implementation of OpenMP can reduce the typical overhead by having the parallel region encompass the whole main loop and partitioning the child loops statically. We apply this method within a variety of software applications (SELF, HIGRAD, CLAMR) to investigate speed-ups due to reductions in OpenMP overhead, thread starts, and thread waiting times by the implementation of high-level OpenMP.
Climate Relevant Aerosol and Gas Phase Species from Combustion Sources

Ambient air quality is impacted by diverse sources, both natural and anthropogenic. Recent evolution in aerosol and gas measurement techniques have allowed for more accurate measurements, particularly with optical techniques. To better understand air quality impacts related to combustion emissions, measurements with several techniques including a system of gas analyzers to measure NOx and a custom controlled relative humidity (RH) nephelometry system to measure light scattering as a function of RH. We used two techniques to measure NOx: light absorption at 405 nm and a traditional chemiluminescence monitor. The method of chemiluminescence uses the reaction of NO and O3 to produce excited NO2, emitting measureable radiation. The absorption method relies on a comparison of visible light intensities with and without NO2 present. To detect aerosol hygroscopic response, a controlled RH nephelometry relies upon the direct measure of light scattering using two nephelometers—one at dry conditions and one at a controlled high RH. In this analysis, we characterize detection limits, determine any interference, and examine measurements of combustion sources. Much of the initial effort has been instrument characterization in collaboration with LANL researchers. Ambient NOx data near Los Alamos and Socorro, NM showed that average NO2 levels are well below national standards. Ambient events in Los Alamos have yielded interesting observations regarding local air quality and instrument response to combustion sources such as smoke from the Dog Head Fire (June 2016), Independence Day fireworks, and influences from a nearby natural gas-fired furnace. The fireworks showed an increase in light scattering coefficient by a factor of 10 with strong suppression of particle hygroscopic response that persisted until morning. A series of combustion experiments is underway to characterize the impacts of burning southwestern biomass.
The modeling of the detectability of special nuclear material (SNM) at ports and border crossings requires accurate knowledge of the background radiation at those locations. Background radiation originates from two main sources, cosmic and terrestrial. Cosmic background is produced by high-energy galactic cosmic rays (GCR) entering the atmosphere inducing a cascade of particles that eventually impact the earth’s surface. The solar modulation potential represents one of the primary inputs to modeling cosmic background radiation. Usoskin et al. formally define solar modulation potential as “the mean energy loss [per unit charge] of a cosmic ray particle inside the heliosphere...” Modulation potential, a function of elevation, location, and time, shares an inverse relationship with cosmic background radiation. As a result, radiation detector thresholds require adjustment to account for differing background levels, caused partly by differing solar modulations. Failure to do so can result in higher rates of false positives and failed detection of SNM for low and high levels of solar modulation potential, respectively. This study focuses on solar modulation’s time dependence and seeks the best method to predict modulation for future dates using Python. To address the task of predicting future solar modulation, the authors utilize both non-linear least squares sinusoidal curve fitting and cubic spline interpolation. The curve fitting process employs and compares three different data range selection processes to identify the one that produces the most accurate localized curve. Initial results suggest that interpolation performs superiorly in both speed and accuracy when predicting solar modular on dates within the data set, while curve fitting returns more accurate predictions on future dates.
Drainage Pattern as Proxy for Lithological Constraints

Evaluation of stream drainage patterns provides a viable option for geologic characterization for setting where only topographic information is available (e.g., denied access locations). The past 60 years has seen considerable work in the field of categorizing river drainages, with progression from understanding stream orders (Horton 1952, Strahler 1956) to first order drainage patterns (Esterbrook 1965), and the observation that rivers with varying degrees of dendritic drainages patterns (i.e. course to fine) was controlled by underlying lithology, sediment budgets, and climate (Way, 1978). This early work, however, was strictly qualitative and more definitive quantitative analysis has waited for the advent of high resolution Digital Elevation Models (DEMs) and fast computing resources to undertake the data-intensive analysis required to assess landscape-scale lithological parameters of the bulk surface composition. Here we show first steps in developing a quantitative approach to understand drainage patterns. We use a topography and fluvial transport model TISC (Tectonics Isostasy Surface Transport and Climate, Garcia-Castellanos 2006) to create simple modeled topographies and allow drainages to develop methodologies to quantify drainages with differing erodibility parameters. We compare two methods: 1- mean drainage linkage angles of a given location and 2 - fourier power spectra to determine quantitative differences of topographies. The use of drainages patterns to constrain surface geologic characterization has important Global Security applications in that it provides a way to construct plausible 3D Geologic Framework Model (GFMs) for locations where access is limited or denied (e.g, candidate foreign test sites). The resulting GFMs provide the numerical framework for shock physics and gas transport modeling which has important Fossil Energy and Global Security applications.
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SuperCam, a stand-off instrument to be launched on the Mars 2020 rover, is currently under construction at LANL and in Toulouse, France. SuperCam’s instrumentation suite includes a Raman spectrometer. Raman spectroscopy is a technique that uses inelastic scattering of light to observe rotational, vibrational, and other low-frequency modes of a system. Raman is often used to identify chemical structures. The spectral range is capable of characterizing both organic and inorganic species. As part of a larger calibration effort, fifty one minerals, relevant to the geology of Mars were analyzed by a preliminary version of SuperCam’s Raman instrument. For each mineral, Raman scattering cross sections were identified using online databases and through literature searches. Twenty seven of the fifty one samples were proven to have bond patterns and vibrations consistent with these resources, i.e., they were labeled correctly. For example, the carbonate family all had their primary vibrational mode, v1, near 1000 cm⁻¹, which correctly corresponds with the literature. In order to distinguish minerals within families first peaks must be compared. For example Siderite has a peak at 500 cm⁻¹ which is not close to any other peaks. Secondly, in order to differentiate peaks that are very close, the distinguishing capability must be less than 10 cm⁻¹. The resolution is currently not accurate enough to handle such closely placed peaks. Hydrated minerals or minerals with OH groups showed characteristic water and OH peaks. Several minerals were either mislabeled or were inhomogeneous and the target mineral was not analyzed. It was also shown that certain minerals do not display Raman spectral features. Future work includes enlarging the calibration database with additional minerals.
Living at the Lands: Understanding Pueblo Fieldhouses on the Pajarito Plateau

Archaeologists define fieldhouses as small, one-to-three room structures that Ancestral Pueblo people constructed using shaped and sometimes unshaped tuff blocks, and usually, have a hearth feature inside. They are the most ubiquitous archaeological site type on the Pajarito Plateau, and there are two widely held assumptions regarding why people built them. First, fieldhouses were related to agriculture as they were constructed to minimize the costs of transportation to and from pueblo villages, serving as temporary shelters while farmers extracted maize and other agricultural resources. The second assumption is that their appearance and growth in numbers is associated with population aggregation as a need for food resources intensified as people coalesced together living in larger pueblos. The goal of this research poster is to examine both assumptions using fieldhouse data collected by Los Alamos National Laboratory archaeologists over the past 20 years. I present preliminary results of a fieldhouse context project that begins to examine fieldhouse variability during the Coalition (A.D. 1200-1325) and Classic periods (A.D. 1325-1600). I consider the function, duration of use, and if the distance from fieldhouses to pueblo villages increased or decreased through time. To accomplish this, I developed a fieldhouse database using Geographic Information Systems (GIS) that included artifact (ceramics and lithics), pollen analysis, and chronometric data from fieldhouse sites within the LANL footprint. The results of this pilot study will hopefully fill in missing gaps within the fieldhouse literature, and I can begin to address questions concerning the social processes of prehispanic population size, settlement patterns, and agricultural systems during a critical time in Ancestral Pueblo history.
Snow impacts earth processes by insulating frozen ground in the winter, replenishing ponds, wetlands, and soils in the summer. Changes in snow depth and snow density, due to climate warming, have positive feedbacks that could potentially result in major vegetation and water cycle changes across the Arctic. The Next Generation Ecosystem Experiments (NGEE-Arctic) project analyzes snow depths and properties in a watershed on the Seward Peninsula, Alaska to monitor changes from year to year. In analyzing NGEE data snow water equivalent (SWE) was calculated using snow depths and densities collected in the field. SWE was plotted against a generalized vegetation map (30-meter resolution) of the area. The map indicates four main vegetation types including: Alder-Willow Shrub, Mixed Shrub-Sedge Tussock Tundra-Bog, Sedge-Willow-Dryas Tundra, and Dryas/Lichen Dwarf Shrub Tundra, which were assigned based on field observations and remote sensing. Comparing these parameters a tentative relationship was found between Alder-Willow Shrubs having higher SWE and sedge/tundra having lower SWE. This relationship suggests that if snow accumulation were to change, it could impact the ability to sustain certain vegetation types. The data used to observe these relationships may have been skewed by thawing and refreezing, potentially resulting in a shallower snow depth reading from frozen layers within the snowpack. Also some of the sample sites were located on a transition of vegetation types. A higher resolution map could more accurately portray the relationship between SWE and vegetation type. Monitoring alterations and abundances in vegetation types in the Arctic must be done to understand how snow and vegetation interact with climate change in real time. This data will be used to create parameters used in Earth system modeling. NGEE-Arctic will continue to analyze snow data and earth processes to improve on fine, intermediate, and global scale Earth System Models.
Demonstrating Effectiveness of Soil Vapor Extraction at MDA-L

The Los Alamos National Laboratory (LANL) stored Volatile Organic Compounds (VOCs) in shafts and pits at Ta-54 Area L from the early 1960s to 1986. The containers in which the Compounds were kept have deteriorated, causing a leakage of VOCs in the gas form. According to national EPA and state laws and regulations, this leak could impact groundwater resources under Los Alamos. For this reason, LANL has installed two Soil Vapor Extraction (SVE) units which are running full time to reduce concentrations in the plume and learn more about how the plume responds to SVE treatment. These units pull subsurface gas from an open interval spanning 60 to 200 ft deep and impact an area out to a radius of about 150 ft wide. After approximately three months of running the SVE units the data collected from monitoring boreholes at the site displayed that the levels of VOCs are decreasing dramatically in certain areas but less in others; this could be due to a variety of factors such as rock permeability, asphalt covering the ground, or how close the SVE units are to the monitoring boreholes. The installation of the SVE units has proven to be effective; however, the data collected show that the area covered by the SVE units is not large enough to fully envelope the area of the leak.
Boron, in the form of borate, is an important prebiotic agent capable of stabilizing the formose reaction. The formose reaction produces early-life sugars, like ribose and various pentoses, from formaldehyde via aldol reactions. As an evaporite, borate could provide evidence that bodies of liquid water once existed on Mars. ChemCam is an instrument onboard the NASA Curiosity Mars rover that uses the laser-induced breakdown spectroscopy (LIBS) technique to evaluate the elemental composition of rocks on Mars. The ChemCam standard database was searched for entries with detectable boron peaks, yielding 31 spectra. Due to interference from a nearby Fe peak, the Fe abundance must be low for a B peak to be visible. The B peak is present in 22 ChemCam observations with <6wt% FeO. A sample set of known varying boron concentrations diluted by terrestrial basalt has been measured using the ChemCam engineering model at LANL. The B peaks of the resulting lab spectra and the 15 spectra from the ChemCam standard database were fitted with a lorentzian peak model using MATLAB. A calibration curve, produced using the B peak areas and the B abundance in the samples, allows us to calculate the abundance of B in Mars targets. The detection limit in the lab of Fe-free samples is 10 ppm. The detection limit was calculated to be 0.56% in iron-bearing targets. Boron has been detected in Fe-free calcium sulfate veins on Mars but it is below the level of quantification. Future work will involve creating a new calibration curve using samples of borax mixed with calcium sulfate. This new calibration curve will allow for a more accurate evaluation of the boron concentration within the calcium sulfate veins.
Understanding Manganese Observations with ChemCam Across Curiosity’s Traverse on Mars

Recent results from the ChemCam instrument on the Curiosity Mars rover have found high concentrations of manganese in rocks in Gale Crater. On Earth, high deposits of manganese did not appear in the geological record until the atmosphere became oxygenated. Manganese oxides can only form if there is liquid water and strongly oxidizing conditions. Thus, Mn oxides are a strong indicator of environmental redox conditions. The goal of this project is to understand the geological context of high manganese targets across Curiosity’s traverse over sols 778-1384. Rock composition data was obtained by the ChemCam laser induced breakdown spectroscopy (LIBS) instrument. All 477 rocks targets along Curiosity’s traverse during the selected time period were analyzed for manganese abundance, which represents a total of 3296 sampling locations. Manganese abundance was quantified using a univariate model of manganese peak area develop by Lanza et al. (2014). 0.3% of the sampling locations were found to have ≥3 MnO wt%, well above the Mars average of 0.4 MnO wt%. Relationships between manganese and major and minor elements were also assessed. These samples typically show high iron, sodium, aluminum, and lithium, and low silica. High manganese oxides targets were also analyzed for compositional depth trends; only three targets showed evidence for changes in Mn abundance with depth, suggesting that these are not surface-related features. Images of the highest Mn targets were analyzed for texture, grain size, albedo, and whether manganese was associated with a particular geological feature, such as an individual mineral grain. High Mn was found in a diverse range of rock types, including conglomerates and crossbedded fine-grained sandstone. The high manganese targets were primarily found in the Stimson Formation, the youngest geological formation identified in Gale to date. Work is ongoing to better constrain the geological processes responsible for these deposits of high manganese.
In Situ Hydrogeochemistry to Understand Current and Future Arctic Hydrology

As a changing climate continues to impact the terrestrial arctic, predicting the uncertain future of this landscape has become an essential part of today’s climate research. The Next Generation Ecosystem Experiments (NGEE) Arctic project aims to investigate hydrochemistry in the Seward Peninsula of Alaska to determine how climate change has impacted a warming polar region. Many geochemical processes contribute to the regional hydrology, which further impacts nutrient production in soil environments and determines the release of greenhouse gasses from thawing permafrost, namely CO2 and CH4. The chemical parameters of a region indicate whether an environment is oxidizing or reducing, which has direct implications for the types of greenhouse gases stored and emitted. In order to understand the geochemistry of the arctic, we measure various analytes, including ferrous iron and sulfide. In situ testing for these chemical proxies has proved to be important in the analysis of the hydrologic and pedologic responses to thawing permafrost. Because the arctic presents unique challenges to fieldwork, we locally tested and compared field methodologies to lab measurements in order to determine which methods most accurately represent conditions at the time of collection. From this testing we determined the best approach for collecting geochemical measurements in Alaska, taking into account challenges scientists face in the arctic such as frigid temperatures, the remoteness of locations studied, and the lack of scientific infrastructure. The selected methodologies were applied to a field campaign in mid July to better determine oxidation and reduction conditions in the Seward Peninsula. Data collected will be used to better inform climate models of arctic ecosystems by parameterizing the impact of climate change on arctic hydrologic conditions.
The critical need for advancing Carbon Capture, Utilization & Storage (CCUS) technology has recently been reaffirmed in the US-China Joint Announcement on Climate Change. The Ordos Basin ranks first in China in its coal, coalbed methane, and natural gas reserves, and ranks fourth in its oil reserves. As of January 2014, approximately 155,000 tons of supercritical CO2 has been injected into a Triassic-to-Ordovician siliciclastic reservoir at 1,690–2,453 m depths. Interestingly, pressure drop was observed at the wellhead of the injector. After 3 years, seismic data and 4 short-duration CO2 injection tests suggest that almost 80% of the CO2 migrated into the Liujiagou sandstone formation at the top of the reservoir. Because both surface reservoir analogs and well logs from the injection and monitoring wells suggest strong reservoir heterogeneity, we developed simple geologic models using seismic, well logs, and core data while accounting for facies and sub-facies heterogeneity. Eclipse compositional simulator was used to model CO2 injection for 3 years. This model was history-matched to the 3-year production data, before it was used to explain observed pressure response at the injector and to fit the CO2 plume shape. Simulation results indicate that both layer-cake and two-point statistical models were unfit (not explaining the phenomena) and more sophisticated modeling methods are needed to better represent the facies distribution described in existing literature.
Cuticular Conductance in Juniper and Oak

Stomata are microscopic pores found on the epidermis of leaves. The stomata control the gaseous exchange of carbon dioxide and water throughout the plant, essential for photosynthesis to take place. Stomatal conductance is the rate at which this exchange between water and carbon dioxide occurs. In a healthy plant, the stomata remain open when exposed to sunlight to allow photosynthesis to occur. However when leaves dry out in drought conditions, they close their stomata to prevent more water loss as a survival mechanism. Despite the assumption that the stomata are closed during drought, there is typically still some water loss through the cuticular tissue of the plant. This is known as the cuticular conductance rate. This unintended water loss can be the reason that plants die in drought. We recorded the rate of water loss due to cuticular conductance in two Southwestern species of trees Juniperus monosperma and Quercus gambelii; commonly known as one seed juniper and gamble oak at two different temperatures: 20°C, and 40°C to produce a low and high evaporative demand. The original hypothesis was that the water loss rates would be higher at 40°C, due to a higher evaporative demand. However, previous results showed that water loss rates were significantly higher at 20°C. We hypothesized that in these species the stomata remain open at 20°C, allowing larger amounts of water to escape via the stomata. To test our hypothesis, we measured stomatal conductance simultaneously with water loss rates using a Licor Portable Photosynthesis System, and a SC-1 Leave Porometer several times per day on three branches from each species. Each time we recorded the mass of each branch, the tree lost mass due to water loss. Our preliminary results suggest that Juniper kept the stomata open initially at 20°C.
Enhanced Global Seismic Resolution using Proposed Undersea Cables

With the exception of a few isolated, near shore deployments of Ocean-bottom seismometers (OBS's), most seismic instrumentation is located on land, although two thirds of the Earth's surface is covered with oceans. Most large earthquakes are unevenly distributed along the Earth’s subduction zones; hence, large areas of the Earth are unevenly sampled in terms of seismic rays. The goal of this work is to produce a comparison of seismic ray coverage of the Earth with today’s seismic stations to that which might be possible in the future, if densely-instrumented transoceanic cables are deployed. Our work is motivated by the planning of a Joint Task Force under the UN that is proposing to integrate seismic sensors at ~75 km intervals into the next generation of Oceanic telecommunication cables. These sensors offer the potential to improve global geophysical models as well as reduce event detection thresholds and location uncertainties in poorly characterized regions. Data coverage is first estimated using an infinite-frequency ray-tracing utility (Pcalc) that has been developed for supporting the LANL nuclear explosion detection mission. We also use a spectral element method code (SPECFEM3D) to compute finite-frequency kernels that include the first order of scattering produced by 3D anomalies. Theoretical P-wave raypaths from 1668 earthquakes to 4421 seismic stations were used to produce global raypath density images in the crust and mantle. We present the improvement in ray coverage achieved at crustal and mantle depths by the addition of 1382 sensors along the telecommunication cables and we discuss the areas in which our models and earthquake characterization benefits from these proposed instruments.
Using Wildfire Models to Understand Fire Behavior

Fire is a critical natural process that cleanses the environment, allowing for rebirth; but fire can also threaten human lives and destroy towns. Understanding fire behavior is key to protecting infrastructure and safely managing fire to regulate ecosystems. Using detailed fire models improves basic understanding of how fire spreads and reacts to different conditions – wind speed, fuel moisture and density, topography, etc. FireTEC is a computationally intensive fire model that runs on high performance computing (HPC) systems and represents much of the complex physics of fire. It can be used to learn about fire behavior by isolating different parameters and analyzing their impacts on spread rate and wind patterns. While FireTEC resolves many details, it also requires large computing resources and runs much slower than real time. In order to build a fast-running model, QUICFire, representation of the physics and computational algorithms must be significantly simplified. Optimizing QUICFire so that it accurately demonstrates fire behavior, and runs close to real time, on a regular desktop, and larger domains, requires knowledge of the most basic and influential fire behaviors. 2-D and 3-D visualization allows for analysis and comparison between the two models. Both FireTEC and QUICFire are coupled with atmospheric models (HIGRAD and QUIC), to capture the interactions between fire and the atmosphere, including the effects of the fire-induced buoyancy on the surrounding flow field. However, QUICFire is unable to resolve all details for the physical processes including the separation between convection and radiation heat transfer to the unburned fuel. A tool like QUICFire could eventually be used in the field to help fire management predict spread and better manage fire. Ultimately, there will be many different tools, with different purposes and strengths in computational power, run speed, required resources, and detail, resulting in a better understanding of fire.
Changes in Composition of Murray Bedrock in Gale Crater, Mars

The NASA Mars rover Curiosity is investigating Gale Crater and its 5 km tall central sedimentary mound, Mt. Sharp, to study the habitability of ancient Mars. ChemCam is an instrument onboard Curiosity that is used to determine the elemental composition of Martian rocks and soil. ‘Murray’ is a finely laminated lacustrine mudstone geologic unit of Mt. Sharp. The change in the elemental composition of Murray was monitored as the rover traversed vertically up Mt. Sharp from sol (martian day) 1271 (Naukluft Plateau and Helgas localities). These data are compared with Murray data along the traverse since sol 700. Currently, 120 observation points have been collected by ChemCam on Murray targets, although the number of data points will likely increase as the rover continues on its traverse. Ca, Mg, and Al have had the largest variation along the traverse. For example, Murray in the East Naukluft Plateau region seems to represent a new Murray composition, with higher Al than most Murray targets. So far, the data show that the changes in composition correlate with elevation. Data from locations in East Naukluft and Helgas are at the same elevation (~ -4426m) and for each major element besides Ca, composition is consistent regardless of lateral location. Also, Si and Al are both correlated with elevation. An increase in alumina could be consistent with an increase in chemical alteration of the source materials that formed Murray. Changes in Murray will continue to be monitored as the rover approaches the hematite-capped ridge 3 km to the southeast and 250 m higher in elevation relative to the rover’s current position.
Circulation in the Ecologically Protected Lau Basin

The Lau Basin, located in the South Pacific, north of New Zealand and East of Fiji, is a back-arc basin with active hydrothermal vents and volcanoes. In September 2015, the New Zealand Ministry for the Environment announced the new Kermadec Ocean Sanctuary in the southern portion of the basin. The sanctuary, which covers more than 620,000 square kilometers, is the world's largest protected marine environment boasting endangered species from turtles, whales, and seabirds to corals, shellfish, and zooplankton. Though protections are in place for the ecological residents of the basin, little is known about the fluid circulation that permits such ecological diversity. Whitworth et al. (1999), explored the water-masses associated with the deep western boundary current (DWBC) in the Tonga-Kermadec Trench and found the trench to be a passageway for Circumpolar Deep Water (CDW) into the South Pacific. In this project, an analysis of "Ridge 2000" floats, and Argo floats show intrusion of water from the trench into the basin, potentially providing another pathway of CDW into the western edge of the South Pacific. Using a simple model developed by Stommel-Arons (1960) and expanded upon by Pedlosky (1989) for abyssal circulation, the bulk of the flow pattern observed from the floats is qualitatively described, including the well defined DWBC, first observed in this data, along the Lau-Fiji ridge.
The behavior of fuels in nuclear reactors in contact with water and contamination of legacy production sites have spurred numerous studies on the chemical behavior of actinides in the natural, surface environment, but relatively little is known about actinide (e.g., U, Th) and cladding material (Nb, Ta, Zr) behavior in high P-T aqueous environments. Given the abundance of water in the Earth’s environment and the ability of radioactive materials to heat up this water it has become imperative that we now address fundamental knowledge gaps in the behavior of these elements at high T aqueous conditions. Metals are transported in aqueous solutions in both the form of hydrated aqueous ions (e.g., Nb5+) and in the form of aqueous species (aqueous complexes: e.g., UO2Cl3-); the latter often predominate over the hydrated ions. Consequently, the first requirement for quantitatively modeling the hydrothermal mobility of U and Th is knowledge of the stability of their complexes with the most abundant natural ligands that can be formed with other metals available in the system. The objective of this study will be to determine the stability of U and Th species in Cl- and SO4-bearing solutions at T up to 300 °C using the autoclave solubility method and UV-vis in-situ spectroscopy. The former involves the determination of the solubility of UO2 and ThO2 in solutions containing variable concentrations of Cl- (or SO42-). The latter method involves the recording of UV-vis spectra of U bearing isothermal solutions containing variable metal:ligand ratios.
Microfluidics has multiple applications, but in most applications fluids need to be pumped through microchannels. This is typically done with large peristaltic pumps which limit the miniaturization of the overall microfluidic system. However, pumping fluids in complex microchannels typically require a range of flow rates while maintaining sufficient head pressure. Features like this are not available in common microfluidic pumps. Here we are investigating the development of a miniaturized peristaltic pump that will produce the desired head pressures and range of flow rates that will be suffice for the implementation with complex microfluidic devices. These pumps are designed to operate three microfluidic valves that are opened and closed using a given logic. The valves are actuated using a novel technique using magnetic coupling of permanent magnets, which are embedded with the microchannels. Our calculations show that this microfluidic pump has a wide range of flow rates and large head pressure, while being sufficiently small for integration into microfluidic platforms. Additionally, the pumps are also very easy to set up and use, making them a practical alternative to traditional peristaltic pumps. The magnets are embedded into a laser-cut frame such that the pump’s design is highly customizable, lending itself to a wide range of applications, and giving a single motor the ability to pump in multiple systems simultaneously. In this study we will present the characterization of these pumps in terms of the maximum achievable head pressure and the ranges of flow rates.
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Remote Railroad Bridge Concrete Tapping using Unmanned Aerial Systems (UAS)

Infrastructure spending is such a large component of railroad annual budget that it must be prioritized to ensure both safety and line capacity at all times. Current inspections priorities in the railroad include early detection of concrete pile caps deterioration, caused by the recent increase of car load capacities. Railroad bridge inspectors conduct concrete tapping to acoustically detect deterioration of concrete by sound. However, measuring railroad bridge pile caps’ condition in the field is a challenging task and in general based on the inspector’s experience. The results of this research describe the development, validation, and testing of a remote concrete tapping mechanism enabled by UAS. The new tapping mechanism can remotely impact the surface, record the sounds of those impacts, and post-process the data to inform replacement prioritization. The sounds from the UAS flying near the tapping was removed applying a spectrum subtraction. Tapping sounds were collected at a sampling frequency of 48,000 Hertz and analyzed both in the time and frequency domains. Principal Component Analysis (PCA) of the data enabled the clustering of the different sets of data collected from different concrete surfaces. The results indicate the potential for remote concrete tapping with UAS, enabling cost-effective, safer and more sustainable prioritization and upgrade of railroad bridges inventories.
The fused deposition method of additive manufacturing has largely remained an open loop process in the absence of rigorous process monitoring and diagnostic functionality. By creating a framework that integrates quantitative diagnostic tools whose measurements are coordinated with the printing process and the system which commands the printer hardware, this paper demonstrates the feasibility of closing the loop in additive manufacturing systems. Specifically, this paper introduces the use of a piezoelectric transducer embedded in the extruding tool head as a means of detecting filament bonding failures introduced by manipulating print bed temperature during the build process. Furthermore, this work demonstrates the capability of correcting filament bonding failures (introduced by the above method) that occur near the printing surface of the part. By demonstrating the detection and correction of filament bonding failures in situ, this work provides a foundation for closed loop control of the fused deposition modeling process that may be adapted for other additive manufacturing processes in future work.
Designing Containers for Glove Box Use and Constructing Muon Radiography Detectors

The container design project is based on the need of a container for use inside glove boxes at the TA-55 plutonium facility. The ideal container will enclose nuclear material and keep at least 95% of contents inside when dropped from a height of 12 feet and exposed to temperatures of 500°C for 2 hours while preventing water ingress of more than 50 cc when submerged under a six inch water column for two hours. The container must maintain integrity under these conditions while allowing hydrogen gas generated by the contents to be released and retaining plutonium in the form of oxide aerosolized particulates. A 3D modeling program (SolidWorks) was used to generate prototype designs of potential candidates of the container so that initial testing of the requirements can be performed and user feedback may be obtained. The muon detector construction project is based on the need to determine whether or not iron supports exist inside the dome of the Cathedral of Santa Maria del Fiore in Florence, Italy. In order to analyze thick materials, such as the dome of the Florence Cathedral, deeply penetrating muons can be used to infer internal structure based on the analysis of scattering events inside the material. A drift tube detector, made up of an assembly of smaller drift tube modules, is used to measure the incoming trajectory of muons and another for the trajectory of the muons upon leaving the material in question, allowing for the scattering angles to be determined. The construction of these detector modules consisted of cleaning parts, assembling these parts, leak testing evacuated systems, and checking electrical signals so that the final detector assembly is able to locate any iron reinforcements inside the dome of the cathedral.
Preparations to Measure the Size Spectra of Plutonium Process Aerosol

Radiation protection requirements for LANL are specified in 10 CFR 835, where the total individual effective occupational dose shall not exceed 5 rems in a one year period. In regard to the inhalation of airborne radioactive particulates, the dose conversion factor for 0.1 µm diameter Pu-239, is about 3.5 times larger than that for 5 µm Pu-239 particles, the default ICRP (International Commission on Radiological Protection) median particle size. This current work is a description of preparations to measure the size of plutonium aerosol in TA-55. In 1974, samples were gathered at LANL with an Andersen cascade impactor. This air sampler had four stages that could collect submicron aerosol. The planned work will use a new impactor with ten submicron stages (MSP Inc). The impactor will gather radioactive aerosol onto fourteen aluminum foil substrates in a regularly spaced size sequence between 0.01 µm and 10 µm. Preparations include a new IWD for TA-55 and operating procedures for substrate installation and removal. Quantitative analysis of the samples will be done by the LANL HPAL (Health Physics Analysis Lab) in TA-55. However, before radiation counting of gathered samples can occur, the compatibility of the foil substrates with existing LANL methodology must be evaluated. A description of the aluminum substrate and the expected format of the collected particulates must be given to the HPAL manager. Information has been requested about form factor, sample activity, and particulate adhesion. The magnitude of particulate mass loading also affects the alpha spectrum of a counted sample, where the emitted alpha-particle energy is attenuated by interactions with the atomic orbit charge fields of the aerosol particulate matrix. Ongoing experiments with inert test dusts are addressing the mass loading and adhesion concerns.
Development of Methods for Three Dimensional Printing of Low Density Polymers

The capability is being developed at LANL to manufacture advanced low density polymer structural materials using 3D printing. Such structural materials can be used in weapon and other applications where traditional polymer foams have been used in the past. The overall development effort is being led by C-CDE and is a collaboration involving C, Q, T and MST Divisions. In the effort, 3D computer aided design (CAD) methods are used to design the desired material structure. A STereoLithography (STL) file is then generated from the CAD file. The STL file is then used to generate a G-code file that controls the 3D printer. Using this approach, different structures can be rapidly designed, printed and tests performed on them to understand their mechanical response. To date, simple grid structures have been modeled using Creo, and printing of these structures has been demonstrated using a 3D printer in C-CDE. Continued effort is underway to increase the quality and size of the printed structures. Work is also focusing on design of more complex structures, such as honeycombs and other advanced structures. Using this approach, our longer term goal is to optimize the design of these materials by establishing the capability rapidly design, perform structural analysis, print and perform mechanical testing of structures.
The assembly of Radioisotope Thermoelectric Generators (RTG) is carried out at TA-55 in plutonium facility building 5. The assembly process of RTGs begins with individual components being baked out in a vacuum furnace to remove all organic contaminants and water particulates. The thermal jackets and insulated plug get baked for 5 days at 600 degrees Celsius and 10e-5 torr, the baseplate assembly gets baked for 2 days at 200 degrees Celsius and 10e-3 torr, and the insulation disks gets baked for 3 days at 720 degrees Celsius and 10e-3 torr with each of these baking processes occurring at different temperatures. Once the components are baked, they are transferred into an argon filled atmosphere controlled box (ACB) line where oxygen and water are held below 5 parts-per-million (PPM). If any incidence introduces oxygen or water into the ACB where these parts are stored, then the entire production process will be heavily delayed due to the effected components having to be baked out a second time. To prevent such heavy delays, a container must be designed to hold an argon atmosphere that meets the standards for oxygen and water to be below 5 PPM for a minimum amount of time of 30 minutes to transfer materials from one box to another and a maximum amount of time of 4 days in case of an ACB failure.
The fused deposition method of additive manufacturing has largely remained an open loop process in the absence of rigorous process monitoring and diagnostic functionality. By creating a framework that integrates quantitative diagnostic tools whose measurements are coordinated with the printing process and the system which commands the printer hardware, this paper demonstrates the feasibility of closing the loop in additive manufacturing systems. Specifically, this paper introduces the use of a piezoelectric transducer embedded in the extruding tool head as a means of detecting filament bonding failures introduced by manipulating print bed temperature during the build process. Furthermore, this work demonstrates the capability of correcting filament bonding failures (introduced by the above method) that occur near the printing surface of the part. By demonstrating the detection and correction of filament bonding failures in situ, this work provides a foundation for closed loop control of the fused deposition modeling process that may be adapted for other additive manufacturing processes in future work.
Continuous Air Monitors (CAMs) are used throughout Los Alamos National Lab to alert workers of alpha emitting (e.g.) plutonium particles in the air. LANL has purchased several EpeeCAM™ samplers from Bladewerx LLC (Rio Rancho, NM). The Aerosol Engineering Facility (LANL Radiation Protection Services) was requested to test the performance of the EpeeCAM™ in their aerosol wind tunnel. The 2015 EpeeCAM™ (with two O-rings) had aerosol collection efficiencies between 39.2% and 73.6% for flowrates between 1.5 and 6.0 ALPM, at particle sizes of 3.3 µm and 9.9 µm. Fluorescent oil droplet aerosol was generated with a TSI Inc VOAG (Vibrating Orifice Aerosol Generator). These results prompted the manufacturer to inform LANL of a potential leak path that had been designed into the filter housing. The aerosol tests measured the ratio of collected to reference aerosol, showing that almost half the flow was diverted away from the filter. The EpeeCAM™ was then modified by Bladewerx with a third O-ring that blocks off the leak path. The sampler was re-tested with fluorescent 10µm particles from the VOAG. A Laskin nozzle was used to generate 0.55 µm oil droplets, and results from these tests were quantified by mass balance. The 2016 EpeeCAM™ (with three O-rings) had aerosol collection efficiencies between 79.6% and 106.3% for flowrates between 1.4 and 6.2 ALPM, at particle sizes of 0.55 µm and 10.5 µm. The modified EpeeCAM™ therefore increases aerosol collection by about a factor of two. Measured aerosol deposition nonuniformity on the filter was compared to MCNP (Monte Carlo N-Particle) calculations, to estimate that the actual solid angle detector efficiency would vary from 99% to 108% of the ideal. These values of aerosol collection efficiency and actual detector efficiency were accepted by the LANL Health Physics customers.
Non-Destructive Analysis of Mechanical Damage and Corrosion in SAVY Containers

SAVY containers are prone to interior corrosion and are sometimes damaged during normal use and shipping. Non-destructive testing (NDT) for mechanical damage, plastic deformation, and corrosion within SAVY containers will augment current container monitoring procedures. Our user-friendly, automated system offers novel quantitative analysis capabilities to assure the structural integrity of SAVY containers. This system will reduce the average cost and time per inspection. Following a feasibility study, ultrasonic wall-thickness testing and eddy current flaw detection were chosen to comprise the system’s NDT component. Deviations from the wall thickness of a control are strong indications of corrosion. Eddy current technology can detect surface and subsurface flaws, including pitting and cracks. Data will be recorded from multiple ultrasonic and eddy current probes simultaneously while a proprietary mechanical system repositions them over the container’s surface. Ultrasonic measurements will be used to create a color-coded thickness plot for rapid visual inspection, while eddy current analysis generates a quantitative surface map of abnormalities to identify flaws. Currently, container surveillance must be performed in a glovebox by an experienced technician. An automated NDT system will improve worker safety and surveillance cycle efficiency, allowing for unprecedented capabilities in container management. More frequent surveillance of at-risk containers, creation of a detailed record of each container, and long-term data collection for lifetime certifications will now be possible. Our next step is to conduct controlled experiments to characterize the performance of both NDT technologies in a laboratory setting.
Designing and Building a Cryogenic System for the Single Turn Project

The National High Magnetic Field Laboratory (NHMFL) facility at Los Alamos National Laboratory uses very high pulsed magnetic fields to study the effects of magnetic fields on various samples of materials. The Single Turn Project at NHMFL uses semi-destructive magnets to create extreme magnetic fields that exceed 100 Tesla. Visible light spectroscopy is used to measure the fundamental electronic structure properties of the material in the magnetic field. Low temperatures are necessary in the material as the subtle changes in electronic structure can be obscured by thermal smearing. We have been challenged with designing and building a cryogenic system to cool a sample to a sustained temperature of about 4 Kelvin while the single turn magnet is fired. The cryostat uses a vacuum barrier between the stainless steel outer layer and the copper inner layer to insulate the cooled inside environment from the outside environment. Liquid helium is pumped through a heat exchanger in the cryostat to cool the inner copper shield. The challenge was to cool the cryostat using minimal helium as fast as possible. The inner heat exchanger went through many design iterations to maximize the flow of helium and cooling time of the cryogenic system. The final design cools the cryostat from 300 Kelvin to 4 Kelvin in an hour, where previous iterations of the cryostat took around 8 hours to cool. This cryogenic system will be used in upcoming experiments in the Single Turn Project Lab measuring various materials at super cooled temperatures under high magnetic fields.
Fused Deposition Modeling (FDM) is one of many Additive Manufacturing (AM) methods commonly used to manufacture three dimensional (3D) objects. The FDM process melts and extrudes plastics through a heated nozzle and deposits it in a pre-determined geometry in subsequent layers. The rapid cooling and the non-uniform temperature distribution throughout a part can lead to excessive residual strain, deformation, and failure of a part during the FDM build process. Digital Image Correlation (DIC), an optical imaging technique, was used to experimentally characterize and measure the transient mechanical strain fields of parts during the FDM build process. The preliminary results will show, how it is possible to monitor the FDM build process in real-time, and determine the adequacy of a part’s design for AM.
In 2005, hexavalent chromium was discovered in the regional aquifer beneath Mortandad Canyon at concentrations above the 50-µg/L New Mexico (NM) groundwater standard. This contamination resulted from hexavalent chromium discharges by the lab’s steam plant from 1956 to 1972. The Chromium Plume Control Interim Measure is working to prevent the further southeastern plume migration towards the San Ildefonso Pueblo and to design a pump and treat system to remove the contamination from the regional aquifer. As part of the chromium plume characterization plan, monitoring wells were drilled to determine the scale and location of the chromium plume. A series of injection and extraction wells are currently being drilled and constructed to create a hydraulic wall and to hold the plume at its current location. Near the center of the plume, two extraction wells have been constructed and five injection wells are in various phases of construction along the southern rim of the plume. The extracted water will enter ion exchange columns to remove the hexavalent chromium and will then be sent via pipeline to the injection wells. The water will dilute the local chromium concentrations and cause mounding to prevent plume migration. Extraction wells CrEX-1 and CrEX-3 are completed with CrEX-1 pumping water into the ion exchange system. The treatment system is successfully removing the contaminant and the clean water is land applied via water trucks until the piping infrastructure is built and connected to the injection wells. Three injection wells are still under construction with the whole pump and treat system planned to start operating in November 2016. Once completed, the closed system will run continuously for sever.
Microfluidic Aspirators

Our aim was to develop a simple and low-cost ‘microfluidic aspirator’ that could have multifunctional applications. The microfluidic aspirator was designed to have two microfluidic channels stacked on top of each other separated by a thin and flexible membrane. The bottom channel was composed of an inlet with a cross-section that is smaller than that of the outlet. As liquid is aspirated through the bottom channel, it creates a pressure drop and causes the membrane to bulge into the channel. This unique aspiration technique can lead to multiple applications including: (1) Optofluidic lenses; (2) flow rate and viscosity sensing; (3) to create vacuum on a chip; and (4) to actuate membranes for organ-on-a-chip applications. In this work, using a single microfluidic principle to address the above mentioned applications will be presented. Because the membrane bulges into the bottom channel to create a hemisphere, the structure can be used as an out-of-plane micro-optofluidic lens for different optical applications. The bulging height is a function of the flow rate and the viscosity of the liquid. Therefore, the aspirator can be used as a microfluidic flow and viscosity sensor by tracking the changes in the bulging height for a given flow condition. The bulging may tracked by measuring the pressure change on the top channel, which is filled with air. The bulging of the membrane into the bottom channel can create a pressure drop on the top channel leading to a vacuum-on-a-chip. Furthermore, by modulating the flow in the bottom channel one can also cyclically stretch the membranes resulting into a novel technique for actuating membranes in micro-physiological systems.
Atmospherically Isolated Transport and Storage Container

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Comparing Reaction Yields of a Critical Assembly Experiment to MCNP6 Simulation

The Flattop critical assembly is a fast fission spectrum assembly located at NCERC at the NNSS. Its design allows samples of actinides and other elements of interest to be irradiated and have reaction yields quantified through gamma spectrometry and beta counting. An MCNP6 simulation and subsequent comparison of yield results is beneficial in order to find potential problems with current nuclear data and better understand the assembly. This paper will outline the results of an MCNP6 simulation and compare the simulation and experimental data of several reaction yields. This comparison will highlight any problems with the nuclear data of the nuclides involved.
The Hyrel System 30 is a 3D printer that allows for easy replacement of print heads, and for up to four print heads to be used at once. The Hyrel uses its ability to switch the print heads to allow for different materials to be printed from one machine with ease, or for multiple materials to be used on one print. Some examples of materials include, plastic, clay, and chocolate. The main goal of this project is to further develop two different methods to print clay using the Hyrel which can then be fired in a kiln, creating a ceramic. The first method is a self-glazing clay mixture. For this, different mixtures will be tested for best results, the current mixture being tile kaolin, copper oxide, and a flux. The second method will utilize the Hyrel’s ability to print with multiple materials by using a glazing material and a clay material. The clay material will fill the inside of the model, while the glaze will cover the entire outside of the model. After both techniques have been developed enough to allow for repeatable results, both models and a basic clay model, will be put through a series of tests. These tests will include: a tensile strength test, a compression test, and an “Iosipescu” shear test, following ASTM standards for all three tests. These results will then be compared to the typical values for these materials to see the effect on the mechanical properties of the material when built by a 3D printer. Future work could include developing models with different combinations of glazes and clays, and attempting to create more complex 3D models.
Extension and Calibration of a Coal Combustion Model

Current regulatory and environmental carbon mitigation goals and time lines require carbon-capture and sequestration technologies on point source CO2 emitters such as coal-fired power plants. Coal-fired power plants have long been the primary energy pillar of industrialized nations, and while reduced utilization is an important target for CO2 reduction, coal combustion remains the most intensive and prevalent point emission source, and represents hundreds of billions of dollars globally in infrastructure that cannot easily be abandoned. As such, it is the most important target for carbon-capture technologies, particularly retrofit technologies. The present work supports near-term deployment of oxy-coal combustion as a CO2 capture strategy through computer modeling. Oxy-coal combustion consists of either high purity O2, or a mixture of O2 and recycled flue gas to burn coal and produce a nearly pure CO2 flue gas for convenient capture. This combustion environment is a radical departure from the air-fired pulverized coal boiler. Exa-scale Computational Fluid Dynamics (CFD) modeling enables low-cost, rapid design in this environment; however, it depends on physically accurate and predictive sub-models. The present work improves the predictive capacity and quantifies the uncertainty of the Carbon Conversion Kinetics oxy-fuel (CCK/oxy) code, a comprehensive coal char conversion model designed to predict coal char burnout in the intense oxy-fuel environment. A recent sensitivity analysis of the CCK/oxy model implicated the char thermal deactivation routine as a key model to accurately predict char conversion, and the present work uses Bayesian uncertainty quantification and calibration in conjunction with literature data to quantify and reduce the uncertainty in the vital annealing model.
Grasp Quality Quantification for Robotic Applications in Plutonium Operations

Los Alamos National Laboratory (LANL) supports a variety of research initiatives to improve operator safety, operation efficiency, and site safety in areas of nuclear weapons manufacturing. Many weapons manufacturing processes at LANL involve fissile materials, which emit ionizing radiation. This radiation can harm operators with prolonged exposure. While working with the materials, criticality must also be considered. While both of these issues are managed through engineering and management controls, these instances can be mitigated in many environments by employing robotic elements in place of human operators. Robots are known for their repeatability, efficiency, and their robustness. To deploy robotic elements to the field, many design and programming processes must be matured to alleviate safety concerns. This problem is addressed using a two-pronged approach. First, design processes were implemented to ensure that the task could be completed by a robotic system. Previously conducted efforts resulted in a custom gripper for storage container retrieval as well as selection of a serial manipulator capable of transporting the containers. After the mechanical selections were made, the programming task was undertaken. The mobile robot and manipulator gripper combination are both controlled by ROS (Robotic Operating Systems). To improve the success rate of grasping containers and to support projects in other locations, technology to recognize when a grasp is safe is needed. Secondly, advanced machine learning techniques were employed in conjunction with pressure/touch based sensors to accurately detect the grasp quality on a targeted object. Machine learning algorithms require training to accurately develop a scoring function that detects the grasp quality on the object. Data was gathered through strenuous testing using typical LANL objects in glove boxes as a proof of concept. These algorithms/sensor combinations developed during the testing can be used in any robotic system with location specific data sets, increasing safety at most locations.
Developing a Lung-on-Chip: Small Molecule Absorption in PU Membranes

One of the challenges of tissue engineering for organ models is the absorption of small molecules by polymeric membranes. This study will investigate the absorption of small molecules into a novel thin and flexible membrane for the development of a miniaturized tissue engineered lung. We are using polyurethane (PU) to make the membranes because PU slabs have been shown to absorb fewer molecules than other common materials in microfluidics, such as polydimethylsiloxane, or PDMS. 15 μm thin PU membranes were fabricated by spin coating (3000 rpm for 30s). In order to characterize the absorption of small molecules into PU membranes, we have designed a set of experiments involving several molecules ranging from 150-500 Dalton. Rhodamine B, Aspirin and Estradiol were selected for their fluorescence, hydrophilicity, and hydrophobicity, respectively. Our design involves placing droplets of solutions of each of these pharmaceuticals onto the membranes, and leaving them at 37°C for varying periods of time. We will report the optimal length of time for the study based on the uptake of rhodamine into the samples, which is observed with fluorescence microscopy. Once an optimal time period has been defined, we will use mass spectrometry to determine how much was absorbed by the membrane. This study will help characterize the application of polyurethane membranes in artificial organ systems for drug development and toxicology experiments.
Residual Stress Measurement of Jet-Engine Bearing Elements Using the Contour Method

Compressive residual stresses provide a well-known advantage to the fatigue life of bearing materials under rolling contact fatigue (RCF), but the stresses change under fatigue loading and may later contribute to failures. Previous measurements of the depth-wise distribution of residual stresses in post-fatigue bearings with X-rays involved the time consuming process of etching to determine subsurface stresses and only in limited locations. By contrast, the contour method determines the 2D residual stress map over a full cross section. The method involves the sectioning of the part using Electrical Discharge Machining, measuring the out of plane displacements of the exposed cross section, and using the afforded field as boundary conditions on a finite element model of the component to back calculate the causative residual stress. For this investigation, the residual hoop stresses in the split inner rings of the main shaft bearing assembly of an aircraft jet engine was mapped using the contour method. Prior to measurement, the full-scale bearing made of hardened AISI M50 was subjected to RCF during engine operation. The unique challenges of the particular measurements are discussed. The tested bearings showed effectively no residual stresses induced by the RCF, probably because they were conservatively removed from service prior to sufficient cyclic loading. More highly loaded specimens will be measured in future work.
This poster discusses how part of a multi-directional conveyor system in the plutonium facility was redesigned due to repeated failures. The new design uses sets of rollers and belts integrated into the existing infrastructure in three sections of the conveyor. The redesign process began with designing a frame that holds the rollers at the proper height, allows for mounting the drive motors, and fits inside the preexisting structure. The placement of the motors and drive pulleys was chosen so that all of the components fit in the space allowed. Belt sizes were selected to provide an appropriate amount of stretch. A stress analysis was performed on all designed components to ensure they could hold up to the applied loads. Portions of the frame and motor mounting brackets were then redesigned slightly to be manufacturable. At the same time, engineering drawings of the sections of the frame that hold the rollers were made with geometric dimensioning and tolerancing and then sent to the machine shop for manufacturing. Along with the frame pieces, other essential components of the design were ordered for the purpose of putting together a mock-up to allow the system to be physically tested. After the system is tested and refined, the design can be finalized and the formal approval process can begin.

Mechanical Design for a Conveyor in the Plutonium Facility
Incorporating Gamma Spectroscopy Capability in the Advanced Experimental Fuel Counter

The Advanced Experimental Fuel Counter (AEFC) is one of the nondestructive assay (NDA) systems developed at the Los Alamos National Laboratory. It is an underwater spent fuel measurement system, which operates in both active and passive neutron interrogation modes. It is used to verify an operator declared fissile mass, initial enrichment, burnup, and cooling time of a spent fuel assembly. It consists of six 3He detectors for total neutron and neutron multiplicity measurements, a spontaneous fission source, 252Cf, for active interrogation, and an ion-chamber for total gamma measurement. The objective of this project is to incorporate a gamma spectroscopy capability into the AEFC system so that the parameters such as initial enrichment, burnup, and cooling time, can be calculated in terms of isotopic ratios rather than the less accurate method of gross counts. Cadmium Zinc Telluride (CZT) detectors were found to be the most suitable for implementation in the AEFC because of their smaller size, higher intrinsic photopeak efficiency, higher resolution, and room temperature operation. Efficiency, resolution, and energy calibration measurements of a CZT detector were performed using low activity gamma sources less than 50 μCi of 137Cs and 152Eu, which showed promising results. At this stage it is unknown how the detector will respond to a large gamma emitter such as 60% burnup spent fuel. The Monte Carlo fuel depletion code, Monte Burns, will be used to simulate the isotopic composition of a fuel, while MCNP6.1.1 will be used to model the AEFC system along with the CZT detector incorporated. Shielding thickness and collimator size for CZT detector will be determined from the simulation results. Finally, the performance of an integrated CZT detector in the AEFC system will be studied and future recommendations about the system design will be made based on the results from both experiments and simulations.
Engineering Design Definition of Hardware for Integrated Research Experiment

The Integrated Research Experimental hardware will be used to study aging and compatibility in weapon materials. Two design definitions are being developed that differ by their internal materials and assembly configuration. Both designs use the same containment system, which consists of end flanges, center tube, valves, and a force device. Valves located on the end of each flange and on the center tube are used for evacuation and gas flow in and out of the system. Attached to the threaded flange is the force device which controls the extent of loading imposed on the internal components. The goal of this project was to develop the two design definitions and establish configuration management in a web-based product data management system. Creo was used to develop 3D models and drawings for the two designs, and Windchill PDMLink was used for configuration management of the design definitions.
In-Situ Inspection for Additive Manufacturing via Laser Ultrasound Spectroscopy

This study presents a new in-process laser ultrasound inspection technique for additive manufacturing. Ultrasonic energy was introduced to the part by attaching an ultrasonic transducer to the printer build-plate and driving it with a single-tone, harmonic excitation. The full-field response of the part was measured using a scanning laser Doppler vibrometer after each printer layer. For each scan, we analyzed both the local amplitudes and wavenumbers of the response in order to identify defects. For this study, we focused on the detection of delamination between layers in a fused deposition modeling process. Foreign object damage, localized heating damage, and the resulting delamination between layers were detected in using the technique as indicated by increased amplitude and wavenumber responses within the damaged area.
Chemical and Radiation-Detecting Emergency Response UAV

With recent advances in unmanned aerial vehicles (UAVs) and other remote technology, it is now possible to analyze hazards without dispatching humans into uncertain threats. The goal is to increase emergency responders’ understanding of a chemical, biological, nuclear, radiological, and/or explosive (CBNRE) accident or emergency by eliminating some uncertainty regarding the environment so they can more safely respond to it. HAZMAT and other emergency responders currently enter the dangerous situations they are trying to fix without enough prior information to know what hazards they face. Tools such as handheld MultiRAE multi-gas monitors are responders’ first line of defense to assess the concentration of significant chemicals in the emergency environment. These require the operators to don complete personal protective equipment (PPE) and go within feet of the hazard, at which point they are already exposed to danger. This could be avoided by integrating existing chemical and radiation detectors and UAVs. To do this, a MultiRAE Pro with wireless transmission capabilities was attached to a DJI S1000 Plus octocopter. It was configured to deliver real-time chemical and radiation data by approaching the ground and leaving a MultiRAE Pro/transmitter payload for long-term monitoring missions. The MultiRAE used for this emergency response UAV monitors gamma rays, oxygen, carbon monoxide, hydrogen sulfide, methane, and volatile organic compounds. The ProRAE Guardian software tracks the six components’ values in real-time and the position of the transmitter in order to provide time-dependent concentration graphs and a geographical map of the readings via Google Maps. A GoPro Hero 3 active camera was also attached to the UAV to transmit real-time birds-eye footage of the mission path. With these tools for analyzing potentially hazardous situations, humans can remain further from potential threats so even even emergency responders can stay safer than ever before.
Mechanical Loading Analysis of Internal Components in Experimental Hardware

The Integrated Research Experimental platform is being developed to study aging and compatibility in weapon materials. Because this device is entirely new, it is extremely important for numerous tests to be run on it, to ensure its full functionality. A feature of this hardware is that it possesses a force plate that is able to apply up to 250 lb of force to its inside components. The goal of the design is to apply loads to internal components in a uniform fashion. While the load applied can be easily controlled, little is known about how the internal components will yield and deform. Analysis is being performed on prototype polymer materials, such as Nylon 6/6 and Polystyrene. Once the analysis method is developed it can be applied to the true weapon material. The loading analysis is being performed with forces of 25.7 and 40.8 lbf at 20 °C temperature. The goal of this study was to assess the design of the experiment and ensure that contact loadings between components are uniform and of the expected values. Preliminary design of the experimental platform was based on a simple 1D approach. In this study a 2D analysis is being performed to account for the 2D geometry of the experiment. Analyses done to date is providing a more detailed understanding of how components will yield and deform in the experiment. The poster will present results from the 2D analysis.
Remote Railroad Bridge Concrete Tapping using Unmanned Aerial Systems (UAS)

Infrastructure spending is such a large component of railroad annual budget that it must be prioritized to ensure both safety and line capacity at all times. Current inspection priorities in the railroad include early detection of concrete pile caps deterioration, caused by the recent increase of car load capacities. Railroad bridge inspectors conduct concrete tapping to acoustically detect deterioration of concrete by sound. However, measuring railroad bridge pile caps’ condition in the field is a challenging task and in general based on the inspector’s experience. The results of this research describe the development, validation, and testing of a remote concrete tapping mechanism enabled by UAS. The new tapping mechanism can remotely impact the surface, record the sounds of those impacts, and post-process the data to inform replacement prioritization. The sounds from the UAS flying near the tapping was removed applying a spectrum subtraction. Tapping sounds were collected at a sampling frequency of 48,000 Hertz and analyzed both in the time and frequency domains. Principal Component Analysis (PCA) of the data enabled the clustering of the different sets of data collected from different concrete surfaces. The results indicate the potential for remote concrete tapping with UAS, enabling cost-effective, safer and more sustainable prioritization and upgrade of railroad bridges inventories.
Automation of MCNP Criticality Benchmark Simulations with Postprocess Analysis

The most recent version of the Monte Carlo N-Particle (MCNP) transport code developed at Los Alamos National Laboratory (LANL) utilizes nuclear point-wise continuous-energy cross-section data in a compact ENDF (ACE) format. The accuracy of MCNP calculations depend on the accuracy of nuclear ACE data tables, which depend on the accuracy of the original ENDF files. There are some noticeable differences in ENDF files from one generation to the next [1], even among the more common fissile materials. As the next generation of ENDF files are being prepared, three software tools called benchmark_runner, check_benchmarks, and analyze_benchmarks were developed to run and analyze output from a large number of MCNP benchmarks (over 1000). The first of these codes is compatible with any of LANL’s high performance computing (HPC) systems that use the workload manager moab. The benchmarks are submitted to the moab client so that any number of jobs may be run in parallel, provided resources are granted. This code is also able to change which cross-section ACE files are used in the MCNP calculations. The second tool inspects the slurm and MCNP outputs and summarizes the current success of the first tool, providing information about the number of successful MCNP calculations, calculations with fatal errors, or calculations that ran out of time on the moab system. This tool also prints out all the unique fatal errors encountered and the last completed cycle for benchmarks that ran out of time. The third tool was used in conjunction with a LANL developed post-process tool, mcnptools [2], to extract output data which was used to pull results from the MCNP calculations. Results will be used to generate regression models of k-eigenvalues as a function of various parameters.
Attitude determination and control enables satellites to perform more diverse missions that require precise pointing for activities such as directional communication and measurements. Star Field Sensor (SFS) attitude determination compares images of stars to an on-board reference catalog to compute the direction in which the satellite is oriented. Within SFS systems, there are two main categories: lost in space and a priori. The research conducted focuses on the former, where no attitude knowledge is available. The goal of this research project was to develop a lost in space algorithm and a search catalog to be used on a LANL-designed nano-satellite. The problem was investigated using Matlab to test potential SFS algorithms, studying real star data collected by the SFS camera. The primary algorithm investigated uses vector angles to generate potential star matches. The 2D projection of the stars onto the camera image plane can be extrapolated into 3D vector space. The unit vectors describing the positions of the objects in the field of view are rotated to match their corresponding catalog stars using an iterative verification process to generate a 3x3 rotation matrix. The equivalent quaternion converts between the SFS coordinate system in which the image objects are defined and the sky coordinates in which the catalog stars are defined, thereby indicating the orientation of the satellite. A catalog of the known stars includes positions corrected for the motion of stars relative to each other over time, in addition to magnitude of brightness, based on Hipparcos Tycho 2 catalog data. Catalog size and memory demands are determined by several factors: sensitivity of the optical equipment, exposure time, processing time, processing time constraints, and the number of objects required to verify a pattern. Our goal is to determine the optimal parameter set for this application.
Los Alamos Neutron Science Center (LANSCE) operates a linear particle accelerator (LINAC) that is used for a number of scientific research projects. Due to the presence of gamma radiation, researchers are not allowed in the beam tunnel during operation. Being that the beam tunnel is inaccessible, an autonomous mobile robot is to be placed in the tunnel, monitoring the accelerator during operation. This robot will present real-time data to an operator from sensors such as a color camera, thermal camera, microphones, and muon detectors; acting as eyes and ears to the user. Localization is a fundamental step in autonomous navigation of mobile robots, answering the “where am I” question. For this project, an Extended Kalman Filter (EKF) algorithm is implemented as a positional estimator. The EKF relies on an odometric motion model to predict the robot’s position and LIDAR measurement data to update the robot’s position. The measurement model is based on features extracted from the LIDAR point cluster using the split and merge algorithm, and the nearest neighbor algorithm associates the features to an a priori feature map of the beam tunnel. The predicted and measured positions are then joined using a weighted value by means of the Kalman gain. The effectiveness of this localization technique is demonstrated using the LabVIEW robotics simulator.
Mechanical Interaction Between the Insert and Outsert Coils of 100T Magnet

The 100T Magnet is signature magnet of the Pulsed Field Facility at LANL which can produce the non-destructive field up to 100.75T (world record) for ultra-high field research. The magnet consist of two coil-sets, insert and outsert coil-sets. A slight misalignment between the insert and outsert coil-sets will create a significant electromagnetic force between them. This project studies the effect of misalignment and magnetic field amplitudes on the force between the insert and outsert magnets using finite element method implemented in COMSOL Multiphysics software. A numerical simulation model was also proposed to understand the vibration of the insert structure when there is some misalignment. The result of this study could be used to explain the experimental data and enables us to create the threshold for safe operation of the 100T Magnet.
Exploring Detection Limits of Acoustic Wavenumber Spectroscopy for Hidden Defects

Using numerical models, we explored the performance of wavenumber spectroscopy techniques for estimating corrosion size and depth in several simulated aluminum plates. Through a series of simulations, we studied the effects of varying excitation frequency on spatial wavenumber resolution, corrosion depth and diameter effects on wavenumber estimation accuracy, and how overall plate thickness affects wavenumber estimation. We then added varying levels of white Gaussian noise to the simulated responses in order to study how measurement noise affects the estimates for a given plate thicknesses. We confirmed that in-plane sizing resolution improves with increasing frequency, however, the relationship between frequency and accuracy of defect detection is highly dependent on the size of the corrosion and plate thickness, indicating that the common “resolution equals wavelength” guideline is insufficient and that all geometric properties must be considered together when determining the expected performance of a wavenumber imaging technique.
Development of a Seismic Sensor Designed to Shut Off Power in a Seismic Emergency

Natural disasters like forest fires and earthquakes are inevitable threats to the Los Alamos National Laboratory (LANL) and pose a serious threat to its nuclear facilities. Preparing for and handling these situations correctly is vital to the safety of Los Alamos and also in keeping a positive view of LANL in the public eye. LANL is regulated by the federal government to implement and maintain specific safety standards. US nuclear facilities are structurally designed to successfully endure any expected earthquake. An additional layer of safety that can be added is equipment that will shut off power to a facility, preventing electrical fires if live wires become shorted. The purpose of this project is to design a device that will shut off power to a facility upon detection of an earthquake of appropriate severity. The device will utilize an accelerometer, which must work in summer and winter conditions and have the ability to sense the low magnitude, low frequency ground accelerations of and earthquake accurately. The sensor data must then be processed with filters and detection algorithms designed to ignore man-made and non-destructive vibrations while triggering, with high reliability, upon an appropriate seismic event. Prototyping was completed with Arduino and Raspberry Pi microcontrollers that were wired to accelerometers, SD cards, and LED indicators. These devices were programmed to practice acquiring data that was then loaded into MATLAB where algorithms for the final device could be developed and tested. The final element of the project is specification of switch gear that will de-energize the facility when necessary. This package can be added to new facilities, as well as equipment such as cranes and elevators, that require this seismic safety feature and would benefit from a safe automatic shut down during a seismic event.
Exploring Multiphase Material Distribution with Acoustic Wavenumber Spectroscopy

This study explores the usage of a steady-state scanning laser Doppler vibrometer (LDV) system for the identification of transition areas between solid, liquid, and gaseous substances in an enclosed container. This technology images lateral surface displacement under the excitation of a single-frequency ultrasonic tone, produced by a piezoelectric actuator. Differences in measured wavenumber at discrete measurement points of a surface scan can be used to detect the boundaries between solid, liquid and gaseous regions of material. We found that the LDV system could be used to compare the relative distributions of solid wax, liquid wax, and air in a cylindrical container based on local wavenumber changes. Through the same methodology, we were able to distinguish the transition between solid and liquid epoxy in a container. Finally, by repeatedly scanning the container as a phase-changing reaction proceeded within, we established that the system can be used to monitor reactions as they progress.
Divide and Conquer: Encapsulation of Small Particles in Microfluidic Droplets

The ability to encapsulate single micro-particles (e.g. bacteria, algae, etc.) inside microfluidic droplets has several applications in biotechnology. However, current methods of single particle encapsulation inside microfluidic droplets are inefficient, especially for particles that are smaller than 10 μm. In this work, we hypothesize that by using a branched channel to distribute optimally diluted particle solutions, it may be possible to improve the encapsulation efficiency. A cross junction of a microfluidic channel network is typically used to make microfluidic droplets, where two opposite inlets are filled with oil and one inlet is filled with the particle solution. The fourth channel in the junction is the outlet, through which aqueous droplets are collected as they are pinched off at the junction by the oil. We integrated a specially designed branched microchannel network at the inlet so that the incoming particle laden solution is divided into four different inputs and is merged with a carrier flow, which becomes the aqueous input for the droplet generator. By dividing the input stream of particles in different branches, we expect the particles to get distributed into the carrier stream. Therefore, when they form droplets the probability of capturing single particles inside single droplets is improved. Such improvement will depend on parameters like the concentration of the particle in the inlet, flowrate of the carrier fluid, and the stability of the overall flow pattern. The objective of this work is to investigate the effect of these parameters on our ability to deterministically encapsulate single particles into single droplets.
Visible Light Communication

We have been developing a visible-light communication system to transmit data through 12 meters of water. This will enable the use of a wireless beam profile monitor at the target location of the Isotope Production Facility (IPF) at LANSCE, as the target location is at the bottom of a water column that provides cooling and radiation shielding for the production targets. The use of visible light is motivated by the poor transmission of radio-frequencies and of infrared light in water. We are using the communication protocol employed by remote controls for consumer electronics such as TVs, and the Arduino electronics platform to enable rapid prototyping. Careful selection of the opto-electronics components has allowed to transmit over our goal distance of 12 meters in deionized water. We present here the technical details and results of this project.
Regional Topological Scanning of an Open Access National Electric Grid Model

Availability of open access electric grid data is a fundamental requirement for Emergency Management and Response (EMR) and other government functions, which are typically hindered by high cost and restrictions from proprietary grid data. Research and simulation are also beneficiary fields that could advance with less restrictions of grid data sources. To address this problem, an open access US grid dataset has been generated using only publicly available sources. The resulting map layers contain 59,361 links (lines) and 47,102 nodes (substations). Using this dataset, executable power flow models simulating electricity flow on the US electric grid have been constructed. The first task is network topology verification. By using computational scanning techniques, scan rulesets were derived and used to detect incorrectly-mapped grid layers, located in the Western WECC and Texas ERCOT regions. The WECC region flagged 499 substations and 12 lines. The ERCOT region resulted in much more substantial flagging with 875 substations and 146 lines. Flagged attributes in both regions were then ranked based on priority level as “High” or “Low”, to partition future verification efforts. All flagged attributes will eventually be verified against openly available utility documents and some may be geo located using satellite imagery. Ultimately, the main outcome from this project is ready availability of a national grid database and map that can be shared among government agencies.
Advanced Sensor Arrays and Packaging

There is often a divide between laboratory-developed experimental technology and commercialization, with packaging and real-world implementation being significant barriers contributing to this technological gap. LANL has been working to develop novel electrochemical sensors for automotive applications for nearly two decades and now has pre-commercial versions of these sensors ready for field-testing. For the automotive diagnostic industry, current state-of-the-art gas sensors use infrared technology, requiring that exhaust gases be removed from the vehicle and transported to a sample cell, where the gas traces from all of the engines cylinders are collected for analysis. This averaging technique is slow and inaccurate, impeding the precise diagnostics of today’s increasingly advanced engine technologies. LANL’s new electrochemical gas sensors exhibit tunable selectivity, allowing multiple exhaust gas species to be sensed within a vehicle’s tailpipe, and stands to eliminate many of the deficiencies of infrared systems by producing a higher level of accuracy in-situ and in real time. However, the temperature, particulate, and size restrictions of in-situ gas characterization necessitate materials engineering in order to develop novel sensor packaging capable of shielding the sensor, while also permitting non-turbulent flow and normal sensor function. Use of multiple sensors presents an exciting opportunity to achieve even higher resolution and sensitivity in complex gas-phase environments. However, sensor arrays present an even greater packaging challenge. LANL is presently developing multi-sensor arrays and working with Rutgers University to produce Bayesian mathematical models capable of deconvoluting signals produced by complex gas mixtures. Such powerful and robust systems have potential uses outside the automotive industry as well, including the detection and identification of explosives for global security applications. Recent advances in electrochemical sensors and application-specific packaging will be presented, along with how this work has enabled real-world field trials testing of LANL safety sensor technology at commercial hydrogen vehicle filling stations in California.
Traditional part inspection, whether at LANL or industry-wide, is performed using Cartesian CMMs with either tactile probing or dynamic scanning. To ensure high-quality part inspection, high-data density measurement sets are performed to properly characterize part geometries. However, this usually employs high-accuracy and highly-sensitive equipment such as hard-contact probing or blue-light scanning. Such technologies, although excellent in their own rights, either cannot produce point-cloud data (CMM) or utilize superficial coatings to ensure proper surface reflectivity (blue-light). To solve these issues, an articulating arm CMM (AACMM) with an integrated laser scanner is used. Laser scanning allows the ability to quickly measure and create accurate, high-density point clouds without contact or surface alteration. When scanning a part, data is acquired from numerous scans of the part surface, thus generating a representative point cloud of the part. Coordinates are then calculated from every noted point via a triangulation method. This allows for a decreased risk of physical damage to “blank” parts throughout the inspection processes and easy digitization of free-form surfaces. Reverse engineering, a major applicatory advantage, is additionally made possible; CAD models and data can be thoroughly acquired from any existing physical artifact. The research presented is to investigate the accuracy, precision, and measurement capability associated with laser scanning to generate point clouds of known CMM artifacts. Additionally, to develop a measurement process for inspection of cast “blanks” prior to initial machining.
High power electron beams have many applications, including isotope production, x-ray sterilization, and radiography, many of which depend on the use of a target to produce the desired spallation end products. This project investigated the design and feasibility of a steel containment for a liquid lead bismuth eutectic (LBE) target. The proposed minimum beam current necessary to produce a sufficient number of particles was 10 mA at 40 MeV. In order to determine if this current was possible and to find a suitable target geometry, finite element analysis (FEA) using Solidworks and ANSYS was conducted. In the analysis, the stresses due to both the pressure stress from the LBE and the thermal stress from the electron beam heating of the steel target containment were considered. This project sought a solution in which the combined stresses that developed in the steel target as a result of the heat and pressure remained below the material’s yield strength and in compliance with ASME pressure vessel code standards. In pursuit of a solution that met this criteria, the beam window geometry, overall target geometry, and eventually the beam current were altered through several design iterations.
Calibrating the RF Resonant Control System for the LANSCE Coupled Cavity Linac

The Los Alamos Neutron Science Center (LANSCE) linear accelerator (Linac) provides high energy protons for scientific experimentation and research. It consists of four Drift Tube Linac cavities and 44 Coupled Cavity Linac modules, operating at 201 and 805 MHz respectively. Protons are resonantly accelerated by radiofrequency (RF) cavities. The operating frequency of the accelerating cavities is determined by their physical size. The coupled cavity Linac accepts 805 MHz RF power, and the cavity must be kept in resonance by a control system which balances the thermal expansion caused by the RF power with thermal contraction caused by water cooling. The temperature of the cavity structure is monitored by thermistors, which detect the temperature of the water at the input and output of the cooling system, and this data is used to control the water valve, opening to cool the system and closing to warm it. The control system must be calibrated regularly to ensure that the cavities are kept at resonance, keeping RF power reflected from the cavities at a minimum. This calibration has not been done since 2009 and needs to be updated. Calibration is done by changing the settings on the resonance control system, and recording, at each setting, the forward and reflected RF power to the cavities, the temperature of the system and the average RF power in the cavity. All data is graphed and the point where reflected power is kept at a minimum is found. Newly calibrated settings are then implemented, and graphs are posted on each module as aids for operators. Results have shown that the current set points for the resonance control system are inaccurate, and demonstrate that more frequent calibration is necessary.
Pulsed Laser Testing for Single Event Effects

A major issue in modern circuit design is the effect of radiation on electric circuits. Radiation can cause either a temporary disruption in the operation of the circuit (commonly referred to as single-event effects) or to rapid degradation due to radiation dosage over time. Modern studies into radiation effects focus on both space and terrestrial environments. In space environments, satellites and spacecraft typically consist of complex circuitry that must be tolerant to the many sources of radiation encountered otherwise the goals of the mission may be jeopardized. In terrestrial environments, due to the constant shrinking of the transistor feature size, circuits operated on the Earth’s surface have also become vulnerable to radiation. To ensure proper operation of a circuit in both environments, it is imperative to accurately analyze the radiation hardness of a circuit. The most common way to ensure radiation hardness is through radiation experiments at particle accelerators. While accelerators typically give a good indication of the real radiation hardness, the lack of availability for testing and inherent drawback of not being capable of fine grain determination of the sensitive regions make accelerator testing problematic. To alleviate this issue, recent work has shown that the use of a pulsed laser can accurately simulate some single-event effects. Compared to accelerator testing a pulsed laser has the advantages of portability and the ability to provide information on the sensitive areas of the circuit. In this poster, we demonstrate the use of a pulsed laser on a LM124 operational amplifier and show that the laser is an effective tool in determining the radiation-sensitive locations of a circuit.
Measurement of Temperature Gradients Resulting from Radioactive Decay of Tritium

Several aluminum tubs at the Weapons Engineering Tritium Facility (WETF) were identified as potentially containing tritium, a radioactive isotope of hydrogen. To reduce the possibility of exposure of workers to this material, the containers have not been opened; instead, the verification of the presence or absence of tritium in the tubs will be based on temperature gradients resulting from nuclear decay of the tritium. The gradients will be measured using eight temperature sensors constructed from thermistors and Wheatstone bridges. To determine whether or not this methodology will be successful, a tub identical to those in question has been obtained and surrounded with multiple layers of insulation. The temperature gradient between the tub and the insulation is measured both when the tub is approximately at ambient temperature and when a known electrical current is passed through resistors inside the container—simulating the heat produced through nuclear decay. Test are ongoing, but results have suggested that the temperature sensors may be capable of measuring nuclear decay in the WETF aluminum tubs in an environment experiencing less variation in ambient temperature. These conditions are possible in the WETF which is designed to allow for more precise control of air temperature. Future tests may involve further insulating the tub to simulate this environment.
Ongoing tests at the Annular Core Research Reactor (ACRR) at Sandia National Laboratories aim to measure temperature and strain in materials exposed to a transient neutron-photon environment. Radiation transport and finite element analysis codes are used to predict the thermal-structural response of test articles exposed in the reactor. Strain and temperature sensors fielded on test articles provide validation data for finite element models, while active and passive radiation dosimetry provides data for MCNP models. Future tests at the ACRR plan to field test assemblies in the Fuel Ringed External Cavity (FREC-II) and expose them to the transient anisotropic radiation field. Experimental and modeling efforts are performed to accurately characterize and map the radiation spectrum as a function of space and reactor pulse time in the FREC-II test cavity. By fielding both active and passive dosimetry in FREC-II, the MCNP model can be calibrated to each of the reactor pulse sizes and shapes. The MCNP model will then provide sufficient data for transient thermal-structural analysis in future studies. The results from the June 2016 FREC-II dosimetry tests aim to characterize the radiation environment in order to calibrate the MCNP models for the DUSTER-II experiment series in September 2016.

Characterization of the Pulsed Radiation Environment in FREC-II at the ACRR
Accounting for Self-heating in High-Precision Pu Density Measurements

Plutonium’s density at LANL is measured by hydrostatic immersion techniques that use Archimedes’ Principle. This density measurement is highly dependent on the characteristics of the immersion fluid being used. We are investigating replacement immersion fluids for plutonium density measurements to obtain more precise density measurements. New fluids are proposed with densities that may vary less, especially in response to plutonium’s characteristics, thus allowing for a more precise density measurement. Our work specifically addresses the self-heating characteristic of plutonium. Currently, we are creating a computer model that will limit the number of physical experiments needed to be performed with plutonium, which is advantageous considering the many hazards associated with working with plutonium. The computer model will also allow for parameter optimizations around the immersion fluid properties, geometry of the plutonium sample and, the temperature to which the system is exposed. This poster will describe the 1) design and additive manufacturing of a sample holder for automated immersion density measurements, 2) production of tungsten samples to mimic the self-heating aspect of plutonium, 3) multiphysics computer model of the density gradients in the fluid due to a self-heating sample and how different geometries affect density measurements, and 4) verification of the computer model using Schlieren flow visualization techniques. The results of this project will decrease the uncertainties in density measurements of plutonium due to self-heating and complicated sample geometries, ultimately supporting applications in new nuclear fuel technologies, power generators for space exploration, and advances in nuclear weapons technologies.
Feasibility of a Plastic Scintillator in Designing a Light-Weight Neutron Rem Meter

In this study we investigated the feasibility of designing a light weight neutron rem meter based on a novel plastic scintillator. Recent developments in plastic scintillator technology have improved their gamma and neutron discrimination properties – an essential capability for success. We have collected pulse height and pulse shape data from a number of different neutron sources using a digital spectrometer. This data was recorded using neutron reference fields where the dose rate is well documented. Using off line analysis tools, we have shown that neutron and gamma discrimination based on pulse shape is achievable even with a modest 40 MHz digitizer. Based on pulse shape, the pulse height spectra have been separated into individual gamma and neutron (proton recoil) components. Calibration of the proton recoil spectra were based on Compton edges observed in the gamma spectra. Efforts are underway to extract dose rate data from the neutron pulse height spectra for comparison against the known dose rates. The eventual goal is to design a probe where the off-line analysis is done in real time.
Treadmill Desks at LANL - Pilot Study

In the United States today about 1/3 of the population is considered obese (Finkelstein, 2009). The 2008 annual health care cost for obesity, in the United States, was estimated at $147 billion a year. Annual health care costs for obese individuals are $1,429 per person more when compared to healthy individuals. Obesity increases risk for developing health issues such as hypertension, coronary heart disease, stroke, type 2 diabetes, and osteoarthritis. Since treadmill desks are a fairly new invention not much research has been done on them. Some of the concerns with treadmill desks are (1) will individuals continue to use them without being reminded to on a daily basis and (2) will it improve an individual’s overall health. Unfortunately it was found that LANL employees did not utilize the treadmill desks therefore no results concerning overall health were found. However, we found that the LANL population does not use the treadmill desk therefore treadmill desk won’t be implemented here at LANL.
Biomagnification of Cesium-137 through Various Trophic Level Sequences at Los Alamos

Biomagnification is a process where the amount of a chemical substance increases as it rises through a trophic level. A trophic level refers to different degrees within the food chain, such as producers, primary, secondary, and tertiary consumers. Cesium-137 has a history of use at Los Alamos National Laboratory (LANL), has a half-life of 30 years, is an analog of potassium, and is known to biomagnify by three times per trophic level. This study reports on the cesium-137 levels of four trophic level sequences: (1) understory vegetation (UV) (grasses and forbs) (n=27) to deer mouse (Peromyscus maniculatus, n=10, whole body) to great horned owl (Bubo virginianus, n=2, whole body), (2) UV to mouse to gray fox (Urocyon cinereoargenteus, n=1, muscle), (3) UV to mouse to bobcat (Lynx rufus, n=1, muscle), and (4) UV to mule deer (Odocoileus hemionus, n=11, muscle) to mountain lion (Puma concolor, n=1, muscle). Data, including soil concentrations, were obtained from samples collected within and around the perimeter of LANL over a four-year period from 2012 to 2015. In general, levels of cesium-137 showed an increasing biomagnification response from UV (-0.00056 pCi/g dry) to mouse (0.014 pCi/g dry) to owl (0.017 pCi/g dry) and from UV to mule deer (0.0028 pCi/g dry) to mountain lion (0.015 pCi/g dry). The levels of cesium-137 in the grey fox (0.00060 pCi/g dry) and bobcat (0.0059 pCi/g dry) did not show a biomagnification trend since their cesium-137 levels were lower than the mean mouse level. All cesium-137 concentrations in soil (0.20 pCi/g dry) and all biota collected within the LANL environment were mostly at undetectable levels (< minimum detectable concentrations), similar to regional background, and/or were far below ecological (soil) and dose (tissue) screening levels that are protective of biota.
In this project our goal was to come up with a way to help train RCT’s and many others in radiation detection techniques. Over the course of the summer we have been working on a survey simulator using python programming. In our simulator the user moves a mouse to simulate the movement of a probe over a “contaminated surface” containing a virtual source. A graphical user interface tracks the mouse movement and the program provides random audible clicks in response to background and source activity. The extent of the “contamination” and its activity are user selectable as is the background count rate but the location of the source is randomly selected by the software. A Poisson interval distribution is used to randomly generate background and source audible clicks. The simulator also provides feedback to the user if the scan rate is faster than the recommended rate. In summary, this program will be a stepping stone in training exercises for RCT’s and many other groups. It will prepare users for the field by teaching them patience and how different hand held detectors are used in a safe environment where mistakes aren’t reprimanded but instead learned from.
Human Health and Safety Considerations for the Design of a Compact Nuclear Reactor

The Advanced Nuclear Technology group (NEN-2) at LANL conducts research, development, operations and training in the application of passive and active nuclear measurement techniques. NEN-2 also supports the National energy security mission through nuclear criticality research with basic research in nuclear chain-reacting systems. This poster is an initial look at the health and safety hazards associated with a compact nuclear power reactor concept. The imagined reactor will be powered by nuclear fission and use highly enriched uranium (HEU) as the fuel. The major hazards, that designers must be most concerned, can be categorized as chemical and radiological. Like all modern power generation technologies, mechanical and electrical hazards can be handled with current industrial safety programs. However, many challenges remain for the successful construction of a new nuclear reactor. By anticipating the major safety and health issues and providing these to the designers ahead of time, the NEN-2 concepts will soon be one step closer to a reliable and durable design.
Items, buildings and materials used in Los Alamos National Laboratory’s (LANL’s) beryllium operations areas have the potential for surface or hidden/entrapped beryllium contamination. Such items are subject to LANL’s Beryllium Protection Program (BPP) release requirements before they can be downgraded to a LANL non-beryllium area, transferred to another U.S. Department of Energy (DOE) facility for non-beryllium use, or to the general public. According to the LANL BPP, if a room has been used for beryllium operations, it is considered contaminated and must go through the release process. Sampling plans for downgrade of beryllium area to a non-beryllium require a statistically based sampling and analysis approach to ensure the area is free of contamination.
Rethinking ExTrain

Principally responsible for many critical laboratory systems, the SAE-2 Work Order & Security Applications team is tasked with supporting a global institution with world-class protection responsibilities. One such application, ExTrain, is familiar to the majority of lab workers. The system stands as a fallback for training content delivery, credit management and access verification for users who do not have access to secured LANL property or the LANL Yellow network. Access to such facilities and systems requires users to have taken specific security courses within the last year. Under normal circumstances, a user is able to authenticate into the Yellow network and complete these training items. However, in the case that the user allows the training to expire, he or she would lose access privileges to the Yellow network and thus would be unable to autonomously regain access through the internal training system. The current solution consists of an external web interface that relies on email and manual data entry, resulting in a standard multiple-hour delay before access is reinstated. By implementing an automated mechanism for fallback credit granting, labor costs are saved by eliminating both the training group’s arduous data entry burden and employees’ wasted time standing helplessly outside of their work areas. Additionally, modifying data storage methods eliminates threat vectors involving the interface between the LANL Green and Yellow networks. Preliminary, conservative estimates of this project’s financial impact show laboratory savings exceeding two hundred and fifty thousand dollars annually.
High-Explosive Inventory Management for Detonator Production

The primary objective of this project is to develop an automated solution for the detonator production (DET) high explosive (HE) inventory control process. The current method for labeling components with Department of Energy (DOE) HE storage and safety compliant metadata required continual relabeling of component containers every time an organizational or storage requirement change was made. This inventory control process is labor intensive, time consuming and puts personnel at risk of ergonomic injury. The DET HE inventory is comprised of approximately 60K components. An idea was proposed to label these components with a barcode and manage metadata changes in the DET Secure Operations Management System (SOMS). Due to cybersecurity requirements and the sensitive nature of HE components, any computerized solution would not be allowed to use common wireless communication protocols such as Bluetooth, Wi-Fi, or a camera. In order to conform to these constraints, I made use of the Intermec CN70NI Mobile Computer, a mobile barcode scanner that lacks all wireless transmission capabilities. The most difficult part of the project was determining how to store data on the scanner, search the data for corresponding information, and then display it to the user. After much deliberation and careful analysis of commercially available inventory solutions for the CN70, I decided that a custom built application would provide the greatest flexibility in customizing specific data field solutions. This application receives all of the necessary data from the CN70’s built-in barcode scanner in addition to a .tab file from the FileMaker Pro database. Once a barcode is scanned, it searches the .tab file for matching data and displays the appropriate metadata to the user. Now DET has a fast, reliable, and dynamic solution for quickly viewing information in the field, can reduce risk to personnel, reduce labor cost, and ensure accurate compliance with requirements.
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Automated Security Test and Evaluation Plan to Support Continuous Accreditation

Information systems are always evolving. Components are added, modified, updated, and removed on these systems daily. New systems are created and configured to solve new problems. With these new additions, come new security risks that must be addressed. Using guidelines and defined values set by the National Institute of Standards and Technology (NIST) and Committee on National Security Systems (CNSS), continuous accreditation must be accomplished to fully implement Risk Management Framework. With this tool, Information System Security Officers (ISSOs) can collaborate on a Security Test and Evaluation Plan (ST&E) with Certification Agents and the Information System Security Manager in real time, thereby allowing for better transparency, reducing the number of duplicate ST&E copies and improved transparency between ISSOs, Certification and Accreditation staff (CAs), Cyber Security Specialists (CSSs), and the Approval Official (AO).
The Viability of HP Web Jetadmin and HP JetAdvantage in the Laboratory Environment

Cybersecurity is a process that has grown exponentially over the years and will continue to do so into the future. One area of this that is often not addressed is that of the network/desktop printer. Printer management and security are becoming more complex and sophisticated as printers are increasingly becoming a vector for cyber-attacks. To address this threat, we were tasked with testing and evaluating HP Web Jetadmin and JetAdvantage for managing and securing printers in the ADX environment. Our presentation will show the results of that testing, some of the conclusions that were drawn from it, and what we think the path forward on this should be.
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The AskIT Service Desk (SD) is the first point of contact for IT-related service requests, problems, and inquiries. SD support is in high demand because their support model relieves other IT service providers from resolving all but the most complex service requests and incidents. The SD also serves as a function for onboarding IT services, meanwhile it helps Laboratory IT customers return to productivity quickly and efficiently. The objective of reporting is to ensure all functions and processes are maximizing customer satisfaction and Laboratory productivity. The Incident Management System (IMS) is the foundational element for improving Information Technology Service Management (ITSM). Without the IMS, managers can only speculate or rely on "conventional wisdom" to make decisions. The IMS supplies operational data, but the ability to generate reports converts data to knowledge and knowledge to actions. Reports are used to; yield metrics to show how the operation is performing, perform analyses to identify the root cause of defects and to eliminate or mitigate the problem, identify areas for automation to improve efficiency, and examine the need to reallocate resources. Without reporting, operations are doomed to repeat the same errors and to work harder and not smarter without many prospects to improve. In an era of declining budgets and the need to improve operational efficiency, improving reporting capability must be a strategic objective.
Effect of Polaron on the Efficiency and Stability of Hybrid Perovskite Photovoltaics

Hybrid organometallic perovskites (HOPs) are promising thin-film photovoltaic materials for multiple reasons including long electronic carrier diffusion length, low electron–hole combination rates, high optical absorption coefficient and cheap processing methods. However, the basic science behind these materials’ synthesis, structure and opto-electronic properties are yet to be well understood. In addition, their unique properties such as I-V curve hysteresis and photoinduced reversible degradation differentiate them from common semiconductor materials. The later is caused by light activated meta-stable trap cites called polarons. These reduce efficiency of the device under illumination and relax in dark, returning the system to steady state. In this work, using density functional theory and symmetry analysis, we investigated the mechanisms of polarons formation and their effect on the electronic property and efficiency of HOP solar cell devices.
In many systems, vital components are manufactured out of polymeric materials. Therefore, it is important to understand how these polymers behave in the various environments they may encounter. One factor governing how polymers behave is the interaction between polymer chains. These complex interactions are influenced by processing history; therefore, differences in manufacturing will result in parts with varied or even unintended properties. In this work, thermal behavior of silicone DC 745 material is studied. Thermomechanical analysis (TMA) determines the changes in sample dimension resulting from changes in temperature, force, atmosphere, and time. This technique can measure thermal events such as coefficient of thermal expansion (CTE), melting, glass transitions, cure shrinkage, and internal relaxations. Using a thermomechanical analyzer (Q400 TMA), preliminary studies determined that DC 745 expands anisotropically when heated. This means that the material has a different CTE depending upon which direction is being measured. In this study, TMA experiments were designed in order to confirm anisotropic thermal behavior in dozens of samples from multiple DC 745 parts of various ages and lots. TMA parameters such as temperature ramp rate and preload force were optimized via a series of experiments to ensure the most accurate and useful data. Additionally, modulated differential scanning calorimetry (MDSC) was used to explore possible corresponding anisotropy in the heat capacity of DC 745. Having a better understanding of this anisotropy will allow for more accurate modeling of systems using DC 745.
Hydrophobic, Heat-Resistant, & Porous Filter Material for Safe Nuclear Waste Storage

The safe handling and storage of nuclear waste is an omnipresent challenge faced by Los Alamos National Laboratory and other nuclear facilities nationwide. Through normal radiolysis and decay processes, the waste in specially engineered containers releases hydrogen gas, which must be allowed to escape the container. This presents the following unique obstacles to the filtration systems in place: 1) they need to allow off-gassing without releasing waste particulate, and 2) must keep water from entering the waste container in the event of a fire in order to prevent possible contamination and criticality events. Our present hydrophobic treatments involving fluorination of copper and aluminosilicate materials are functional up to 400°C, a temperature just short of the Department of Energy's goal of 550°C. We will present our work on new chemical processes and treatments aimed at raising the operating temperature of the filters to 550°C while still exhibiting the desired hydrophobicity and filtering characteristics.
Using a Film Applicator to Determine Platinum Loading for Fuel Cell Electrodes

Most Polymer Electrolyte Membrane Fuel Cells (PEMFCs) utilize platinum as a catalyst for their electrodes. The amount of platinum in the electrode influences the cost, performance, and durability of these FCs. There are several methods to produce FC electrodes, such as hand painting, sputtering, and spraying. In this study, an automated film applicator with an adjustable micrometer film applicator manufactured by TQC is used to produce electrodes. This approach has become an attractive method for mass production of MEAs (Membrane Electrode Assemblies). The film applicator can apply uniform coats and amounts of catalyst to polytetrafluoroethylene (PTFE) substrates at selectable speeds. This study seeks to find a correlation between the applicator’s height and Pt loading. In doing so, we prepared a controlled catalyst ink that is a mixture of platinum catalyst, isopropanol, and ionomer. The catalyst ink is applied to the PTFE substrates while varying the height of the applicator. The platinum loading is determined for each height via X-Ray Fluorescence (XRF). This allows a correlation between platinum loading and the applicator height to be determined, which subsequently allows any desired electrode loadings to be identified by setting the height.
Microorganisms are critical sources for different types of bio-products including biofuels, nutrients, and drugs. Low doses of microwave radiation in the 40 - 46 GHz range have been shown to significantly enhance the growth rate of some microorganisms. Our goal for this project is to investigate the effect of high frequency microwave radiation on the growth conditions for different microorganisms. The power level and the frequency of radiation require in depth research to reproduce previous demonstrations for large scale applications. We want to identify the optimum frequency and power level that may positively influence the growth of a given microorganism. It is important to determine the propagations and penetration depths of microwave radiation through the materials of the bioreactor and the growth medium. Therefore, we first investigated microwave radiation through different materials that are typically used to make bioreactors. Next, we fabricated multiple microfluidic cells containing different thicknesses of water. The power of microwave radiation transmitted through these fluidic channels was measured using a sensor. We varied the distance of the fluidic cells from the source, the thickness of fluid, the type of fluids, and the frequency of the microwave radiation and observed how these variables affected the transmitted radiation. Our measurements showed negligible losses of microwave power while transmitting through an empty microfluidic cell. However, the transmitted power was attenuated by ten times when the thickness of the microfluidic cells filled with water increased from 50 microns to 600 microns. These findings will be utilized to design bioreactors suitable to integrate efficient microwave irradiation for growth enhancement.
Environment-Dependent Interfacial Properties for a Nickel Crystal-Melt System

The rapid solidification of metallic structures through certain manufacturing processes (i.e. additive manufacturing, cast, welding), results in complex changes to the microstructure originating from the rapid heating/cooling rates used for the process. These rates result in a thermal non-equilibrium condition at the crystal-melt interface and affect the interfacial stiffness and energy of the system. The changes in the microstructure are most directly linked to the formation of dendrite structures, typically modeled using phase-field simulations under the assumption of thermal equilibrium. While recent advances have been made to overcome this deficiency within the phase-field simulation methodology, the work presented in this paper proposes an alternative approach using molecular dynamics and a modified capillary fluctuation method to account for the additional contributions due to the non-equilibrium environmental conditions. Additionally, we identify the deviations in interfacial stiffness, free energy and anisotropic parameters of pure nickel sample by applying thermal gradient to a crystal-melt structure originating in equilibrium. The results show a direct relationship between the magnitude of the temperature gradient and the interfacial stiffness, which in turn results in gradient-dependent anisotropic parameters and free energies at the interface.
Fission Fragment Damage Studies

Fission fragment damage was created in 238U and 232Th targets by exposing them to 12.5 MeV quasi-monochromatic γ-rays at the High Intensity γ-ray Source (HIγS) at Duke University. γ-rays of this energy are in the region of the “Giant Dipole Resonance” (GDR) and they can induce fission. A series of targets of 238U and 232Th were exposed to a flux of 80 million circularly polarized γ-rays per second. Exposure was varied by stacking multiple targets in sequence, so as to have the opportunity of correlating damage as a function of fluence. To our knowledge, our samples are among the world’s most highly irradiated samples ever studied for damage due to photofission. The greatest exposure was approximately 7*10¹² γ-rays over an area defined by HIγS gamma-ray beam collimation (16= mm diameter).

After exposure, a preliminary characterization of the targets was performed via scanning electron microscopy (SEM) at the University of North Carolina at Chapel Hill, and potential fission fragment damage was identified. At Los Alamos National Laboratory (LANL), a program is being developed to perform a more systematic analysis of these targets. We are studying the images so as to isolate characteristic fission fragment damage. In the future, the targets will be imaged using electron back-scattering diffraction (EBSD) methods to compare the microstructure of the targets with the locations of potential fission fragment damage. Details of the experiment and proposed analysis will be presented.
Organic Hydrogen getters irreversibly scavenge gaseous hydrogen in closed systems, maintaining very low hydrogen partial pressure where high concentrations of hydrogen could become potentially dangerous. A few successful applications of these getters are in transuranic waste containers and, more recently, in solar cells. 1, 4 bis(phenylethynyl) benzene (DEB) is a commercially produced hydrogen getter. The DEB is not used in its pure form because it does not react with hydrogen on its own. By adding a palladium catalyst on a carbon base, the hydrogenation kinetics increase significantly, even at room temperature. However, the appearance of uncharacteristically low melt temperatures arising from the interaction of the pristine getter and the hydrogenation products is a potential concern. The hydrogenation reaction is exothermic, and depending on the rate of the reaction, it could lead to a significant increase in overall temperature of the environment, potentially leading to a higher mobility in the getter. As the getter molecules move more freely, they are able to migrate away from the catalyst, hindering the hydrogen uptake considerably. We used differential scanning calorimetry, thermogravimetric analysis and IR spectroscopy to analyze mass loss, melt temperatures, and chemical composition of the DEB compound mixed with hydrogenation products to assemble a binary phase diagram for the system. The results characterize the binary phase behavior and how DEB interacts at varying degrees of hydrogenation. Our results show that the melting point of the DEB system is suppressed significantly even at relatively low hydrogenation levels. However, the melting point remains much higher than room temperature.

**Phase Stability of 1, 4 Bis (Phenylethynyl) Benzene (DEB)**

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Determining Differential Curing and Its Effects Within Flexible Cables

By placing an insulting layer of polyimide around and between a conducting copper material, several flexible and electrically conductive systems can be manufactured. In one such application of this technology, both sides of a long, thin copper strip are covered with a layer of Kapton, a thermally and electrically insulating material manufactured by DuPont. In order for the Kapton to adhere to the copper, a 2000 micron thick layer of B-stage acrylate polymer is placed in between each side of the Kapton and copper. The cables are heated and pressed for an extended period of time, at which point the Kapton and copper layers are adhered to one another. At the end of the manufacturing process the delivered cables can have undesirable warping features and can have an excess amount of leakage current. The potential for differential or incomplete curing causing these features within the cables was investigated with analytical spectroscopy. Fourier Transform Infrared Spectroscopy (FTIR) is an analytical spectroscopy method used to determine both the chemical structure and interactions within samples. By measuring the amount of light absorbed, signature groups can be identified within a material. Largely, the acrylate monomer used consists of two functional groups which are both very active in the infrared region of the electromagnetic spectrum. One of these groups is also very active in the polymerization process, while the other is not. This FTIR method can be applied to not only track the conversion process and determine the average pressure and heat-polymerization kinetics, but also track the differential curing and its effect within the manufactured Kapton cables with respect to both press-location and curing time at a given temperature and pressure.
Platinum (Pt) is the state-of-the-art catalyst for both anodic and cathodic reactions that occur in polymer electrolyte fuel cells (PEMFCs). Due to the cost of platinum, fuel cells have been hindered from commercialization. However, one obstacle for next generation fuel cells is to reduce the amount of platinum yet still produce tremendous activity and high durability. In this work we have investigated the effects of aging, with the use of an Accelerated Stress Test (AST) that consists of voltage cycles from 0.6 V to 1.0 V vs. RHE. Furthermore, we studied the electrochemically active surface area (ECSA) of different Pt loadings on carbon. In particular, we used a catalyst supported on a high surface area carbon, XC-72. We tested Pt catalyst of 4.8%, 20%, and 40%. These materials are used in the state-of-the-art PEMFCs. To study the activity and durability of the Pt catalyst, a rotating ring disk electrode (RRDE) system is used in stationary mode. Carbon monoxide (CO) is introduced into the RRDE system because it is adsorbed onto Pt active sites and the ECSA of the catalyst can be calculated. The number of active sites can be determined by measuring the ECSA of the hydrogen adsorption and desorption regions, and CO stripping. Detailed examination of the results reveal that the various loadings of Pt on carbon supported do have an impact on the active sites. This was validated by the decrease in ECSA as the loading of Pt on carbon increased. In all tests, we observed ECSA losses as the number of AST voltage cycles increased.
Examining Materials for Use in Resonant Ultrasound Spectroscopy

Resonant Ultrasound Spectroscopy (RUS) is a nondestructive method used to measure the fundamental vibrational modes of a sample and thereby determine a complete set of elastic constants for that material. Elastic moduli are symmetry-sensitive thermodynamic susceptibilities that connect directly to thermodynamics, electronic structure, and mechanical properties. They can be used to determine other various thermodynamic properties of the material such as the Debye temperature and Grüneisen parameter. The RUS technique involves measuring a material’s mechanical resonances using two piezoelectric transducers: one for excitation and another for detection. The transducers are mounted on a suitable backing material to ensure all of the sound generated is transmitted forward into the sample. The backing material also serves as acoustic insulator, because spurious vibrational resonances and mechanical noise need to be eliminated so that all measured resonances are from the sample. Various glues, epoxy resins, and ceramics are being investigated for this purpose. The equipment also must be suitable for use in a hot glovebox environment as well as very low (~4K) and high (~800K) temperatures. We are investigating the properties of clay components manufactured with a 3D printer. Various tests will evaluate sound attenuation, hardness, machinability, and any anisotropic behavior introduced by the layer-by-layer printing process. The results will indicate how varying different parameters such as printer properties and firing time/temperature affect the ceramic properties.
First Principles Study of O Vacancy Effect on Magnetic & Electronic Prop. in BFMO

In multiferroic materials, a stable electric polarization can be controlled by applying an external magnetic field and vice versa, as mediated by magnetoelectric coupling. Such a unique property makes these systems extremely useful for many technological applications ranging from tunable multifunctional spintronics to magnetoelectric random access memory devices and various kinds of optoelectronic devices. Double perovskite Bi$_2$FeMnO$_6$ (BFMO) is a potential candidate for the highly sought single phase multiferroic system. The large orbital radius of the Bi 6s$^2$ lone pairs is responsible for BFMO to exhibit low symmetries and spontaneous polarization, whereas B-site ordering of Mn and Fe contributes to its magnetic properties. In this work, we study the effects of oxygen vacancy on magnetic, electronic and optical properties of BFMO by performing first-principles simulations using density functional theory within the local spin-density approximation (LSDA) and the LSDA+U method. The calculations were performed on a supercell constructed with eight chemical formula units of BFMO, from which oxygen atoms were removed incrementally. We numerically demonstrated that a strong on-site Hubbard interaction is critical for the gap opening in a pristine BFMO. We then showed that the average magnetization is modified with the increase of oxygen vacancy concentration. From the calculated band structure and optical conductivity, an insulator-metal transition or crossover was identified with the oxygen vacancies in BFMO.
Polyethylene is a simple but robust material used in many applications all over the world and at the Los Alamos National Laboratory. The properties of specific high density polyethylene (HDPE) and ultra-high molecular weight polyethylene (UHMWPE) samples from Polymer Industries have come into question. In order to investigate this, HDPE and UHMWPE were thermally characterized by DSC and TMA to understand the material’s melting temperature, percent crystallinity, heat capacity, and coefficient of thermal expansion (CTE).
There has been tremendous effort to understand damage and damage evolution in OFHC Cu under high rate loading conditions. In the experiments presented in this study, a large bore gas gun was used to accelerate a flyer plate into a stationary target assembly. Photonic Doppler Velocimetry (PDV) was deployed to identify loading and unloading conditions of the target specimen. Also, with the use of a careful geometric target assembly design, soft recovery of specimen was deployed for post mortem characterization. We will present two high rate loading and unloading data sets on two specimens of OFHC Cu. Each of these specimens was subjected to two different loading paths and unloading paths, but yet each specimen was subjected to the same uni-axial tension which is known to create void nucleation. One specimen was loaded at a higher pressure in which is known to produce much more work hardening in the specimen prior to being subjected to the same uni-axial tension as the specimen loaded to a lower pressure. To try and better understand the effects of damage and damage evolution under high rate uni-axial tension, the two specimens were recovered, cross sectioned and polished to explore damage in the area under uni-axial tension. This study is an attempt to further understand and correlate high rate loading conditions to damage. We will present our findings.
2 Dimensional Correlation Fourier-Transform Infrared Spectroscopy (2D FT-IR) is a technique used to measure changes in spectra with respect to a variable, such as temperature. 2D FT-IR is a new technique being implemented at LANL. In order to validate the experimental data gathered using a 2D FT-IR moving window technique, it was necessary to measure a known polymeric property. In this case 2D FT-IR was used to identify a material’s glass transition temperature, an important property in polymers. Glass transition temperature is the temperature at which chain movement in a polymer begins. Physically, this means that the polymer transitions from a hard and glassy state into a rubbery state. In order to validate this method a sample of poly(tert-butyl methacrylate) (PtBMA) was solvent cast into a film on a KBr window. PtBMA was used because the absorbance at 1147 cm\(^{-1}\) corresponds to the C-O ester bond stretch, exhibits a decrease in intensity at the glass transition temperature. Spectra were taken using a Bruker Vertex 80V FT-IR spectrometer with a Simplex Scientific heated transmission cell at temperature intervals of 2\(^\circ\)C from 30\(^\circ\)C to 136\(^\circ\)C. The spectra were then analyzed using the 2D FT-IR technique.

**Measuring Glass Transition Temperature with 2D FT-IR**
For years, additive manufacturing has been making strides to become increasingly cheap. As additive manufacturing develops, it becomes increasingly important to not only design new mechanical tools but also to develop the printing media. For stereolithography, the resin often consists of a monomer, a dye, and an initiator. By exposing the resin to light, the initiator will radicalize, and initiate propagation, while the dye will limit the line width. Of great interest to the community is finding ways of developing resins with unique properties. In this work, a porogen is added to the system to provide new opportunities for materials design with SLA systems. The presence of a porogen means the product can be printed with both mesoscale and nanoscale design elements. By controlling variables such as the amount of porogen added, factors such as the density of the product can be carefully controlled. Additionally, this hierarchical structure lends itself to many applications. For example, a PEG system printed in isopropanol has the opportunity to deliver a low-density bio-compatible scaffold for tissue growth, with the porogen providing plenty of the much desired vascular-like structure. Additionally, the products of such resin can be coated with some sort of functional group to provide even more diverse applications. A sample could be sputter coated with metal, and then heated to have the underlying polymer destroyed. This would leave a meso and nano porous structure of a metal minimal surface. This method can be used to coat the polymer with metals, ceramics, or even a differently functionalized organic layer. Overall, the addition of a simple porogen into a resin mix could dramatically increase the versatility of simple additive manufacturing techniques and allow the development of cheaper specialized materials.
Hollandite Radiation Response

The hollandite structure, $\text{Ba}_x\text{Cs}_y\text{M}^{2+2x+y}\text{Ti}^{8-2x+y}\text{O}_{16}$ ($\text{M}=$Zn$^{2+}$), is one component of a multiphase assembly of ceramics designed for nuclear waste storage. Hollandite can incorporate $^{137}\text{Cs}$ into its tetragonal $I4/m$ structure thereby immobilizing the Cs. Hollandite has fairly high resistance to beta radiation from Cs decay but is vulnerable to alpha radiation from nearby actinide phases. Alpha radiation stability of hollandite doped with Zn has never been measured before and is necessary in order to have accurate models of the material lifetime. Several polycrystalline single phase pellets were exposed to a 1 MeV Kr$^{2+}$ ion beam at room temperature to simulate alpha irradiation present in the waste form. Irradiation damage effects were studied by transmission electron microscopy (TEM) imaging and grazing incidence X-ray diffraction (GIXRD). Complete amorphization was achieved at fluences of $1.5\times10^{14}$ ions/cm$^2$ to $2\times10^{14}$ ions/cm$^2$ (corresponding to 0.302-0.427 dpa) depending on Cs content. Additions of Cs to the hollandite increase the stability thereby promoting higher radiation resistances.
The design of functional nanocomposite systems featuring nanoparticles arrayed in a matrix structure allows for significant enhancement of physical properties in thin films. However, precise and direct control of nanoparticle size, concentration, and distribution has not yet seen the level of success desired. Here, by combining superlattice and vertically aligned nanocomposite (VAN) structures, we have successfully achieved a nanocomposite system consisting of MgO nanoparticles embedded in La0.7Sr0.3MnO3 (LSMO) thin film matrix. The dimension and distribution of MgO particles in the matrix can be tuned by careful adjustment of growth parameters. As a result, this detailed tuning of nanoparticle size and spacing allows for selectable strain in the LSMO matrix, and thus, tunable functional properties. In this study, we have shown strain induced tunable resistivity, metal-to-insulator transition temperature (TMI), and magnetoresistance (MR). These results demonstrate that a new approach to the design of nanostructures with precise control of strain via nanoparticle size and distribution is a viable method toward detailed manipulation of physical properties in thin films, and could be generalized to other complex nanostructures.
In this project, we are developing a separation and purification scheme for the isolation of nanocarbons from detonation soot recovered from high explosives. It is envisioned that the novel nanocarbons will be of value to both the science of signatures and the nanoscience community. Prior work has revealed a wide range of nanostructured carbon’s including nanodiamond, graphitic structures, amorphous carbons which are considered to be the unidentified carbons, several distinctive metals and other metal oxides produced during the detonation of high explosives. To address this opportunity we have developed a multistep purification scheme which will allow us to remove unwanted metals provided by the detonators and separate out various carbons based upon density. A long-term grand challenge in materials science is to understand how to use the lessons and tools of natural reactive processes to produce synthetic and hybrid materials with similar types of tunable and adaptive responses, but tailored for applications in photonics, electronics, sensing or other application areas. Within this framework, and in order to make progress toward the solution-based development of integrated nanomaterials that mimic some of the properties of natural systems, I will investigate scientific topics that include the polymerization of amphiphilic molecules into structure polymers that serve as robust template for organizing metal nanoparticles. There are three unique phases of aqueous extractions with polymers using sodium polytungstate (SPT), zinc chloride (ZnCl2), 1,1,2,2-tetrabromoethane (TBE). Ultracentrifugation of the two aqueous solutions can distribute the carbon’s according to density. From this I plan to characterize the nanocarbons by electron microscopy, X-ray scattering, and electrochemical measurements.
First Principles Determination of Structural Variations in $\delta$-Pu from Self-Irradiation

We used density functional theory to examine the effects of impurities and vacancies in a 108 atom face centered cubic $\delta$-Pu supercell. The impurities considered are radioactive daughters or stabilizers in $\delta$-Pu, which include U and Ga. These impurities were placed at various interstitial sites, including octahedral, tetrahedral, and split interstitial along the (100) direction, as well as substitutional lattice sites. Self-interstitials, mono and di-vacancies were also considered. In addition we examined impurity-vacancy complexes at first and second nearest neighboring distances from each other. Radial distribution functions were plotted to gauge the local structural variations around the defect within the lattice. These local distortions will be discussed.
Magneto-electric (ME) coupling refers to a correlation between the magnetization and the polarization in a multiferroic material or nanostructure, which allows control of the electrical polarization with a magnetic (B) field or vice versa. This effect has attracted great attention due not only to its potential applications in data storage and high speed computing, but also to the underlying physics. Here, we study the second harmonic generation (SHG) signal, as a function of external magnetic field in a high quality 65:35 BaTiO3:CoFe2O4 (BTO:CFO) vertical nanocomposite. By varying the magnetic field from 0 to 0.4 T, we observe a striking enhancement of the SHG signal, explicitly suggesting a strong coupling between the ferromagnetic CFO nanopillars and the ferroelectric BTO matrix.
Resonant Ultrasound Spectroscopy (RUS) is a nondestructive method used to measure the fundamental vibrational modes of a sample and thereby determine a complete set of elastic constants for that material. Elastic moduli are symmetry-sensitive thermodynamic susceptibilities that connect directly to thermodynamics, electronic structure, and mechanical properties. They can be used to determine other various thermodynamic properties of the material such as the Debye temperature and Grüneisen parameter. The RUS technique involves measuring a material’s mechanical resonances using two piezoelectric transducers: one for excitation and another for detection. The transducers are mounted on a suitable backing material to ensure all of the sound generated is transmitted forward into the sample. The backing material also serves as acoustic insulator, because spurious vibrational resonances and mechanical noise need to be eliminated so that all measured resonances are from the sample. Various glues, epoxy resins, and ceramics are being investigated for this purpose. The equipment also must be suitable for use in a hot glovebox environment as well as very low (~4K) and high (~800K) temperatures. We are investigating the properties of clay components manufactured with a 3D printer. Various tests will evaluate sound attenuation, hardness, machinability, and any anisotropic behavior introduced by the layer-by-layer printing process. The results will indicate how varying different parameters such as printer properties and firing time/temperature affect the ceramic properties.
A Multipurpose Test Stand for Scintillator Decay Lifetimes

We built a prototype test stand in order to measure novel scintillator materials’ decay lifetimes. Radiography and imaging are valuable diagnostic tools for studying dynamic experiments, thus new scintillator materials are needed to improve the resolution of the current observational systems. A collaborative effort by the neutron imaging and x-ray radiography teams is underway to study the novel scintillator materials developed at LANL and by outside collaborators. Decay lifetimes are an important characteristic of a scintillator material and so by developing this prototype we have provided an avenue to further scintillator development. We confirmed the effectiveness of this prototype by comparing known scintillator decay lifetimes of LYSO and polystyrene samples. In our proof-of-concept prototype we use an 80 Gs/s oscilloscope. With future implementation of a fully developed test stand, we will use a digital data acquisition system to record complete waveforms to conduct a post-processing analysis of the decay times. Results of the prototype test and potential improvements to final test stand design will be presented.
Using a Film Applicator to Determine Platinum Loading for Fuel Cell Electrodes

Most Polymer Electrolyte Membrane Fuel Cells (PEMFCs) utilize platinum as a catalyst for their electrodes. The amount of platinum in the electrode influences the cost, performance, and durability of these FCs. There are several methods to produce FC electrodes, such as hand painting, sputtering, and spraying. In this study, an automated film applicator with an adjustable micrometer film applicator manufactured by TQC is used to produce electrodes. This approach has become an attractive method for mass production of MEAs (Membrane Electrode Assemblies). The film applicator can apply uniform coats and amounts of catalyst to polytetrafluoroethylene (PTFE) substrates at selectable speeds. This study seeks to find a correlation between the applicator’s height and Pt loading. In doing so, we prepared a controlled catalyst ink that is a mixture of platinum catalyst, isopropanol, and ionomer. The catalyst ink is applied to the PTFE substrates while varying the height of the applicator. The platinum loading is determined for each height via X-Ray Fluorescence (XRF). This allows a correlation between platinum loading and the applicator height to be determined, which subsequently allows any desired electrode loadings to be identified by setting the height.
The durability of the Proton Exchange Membrane Fuel Cells (PEMFC) has been a fundamental barrier in the commercialization of these systems for automotive applications. The Pt electrocatalyst and the carbon support used in PEMFC electrode layers are known to degrade over time in a symbiotic manner resulting in significant performance losses. This study focuses on the durability of the carbon support used in the catalyst layer. The carbon support is thermodynamically unstable under the operating conditions found in PEMFCs and has been reported to corrode especially at the higher potentials (> 1V) encountered during start/stop operations of PEMFCs. The membrane electrode assembly (MEA) used in this study was provided by Ion Power Inc. and consisted of a Du Pont® XL membrane and an advanced Pt/C electrocatalyst from Tanaka. The durability of the advanced carbon support was evaluated using an accelerated stress test (AST) protocol in which the cathode potential was cycled from 1 to 1.5V in a N2 atmosphere at 100% relative humidity and 80 oC. Pt electrochemical surface area and fuel cell performance was tracked with cycling time in order to quantify the degradation rates. X-ray diffraction and scanning electron microscopy studies were performed on both fresh and aged MEAs to track the Pt particle size and catalyst layer thickness, respectively. The degradation rate of this advanced carbon support will be compared to previous data obtained on standard high and low surface area carbon supports. It is expected that the advanced carbon support will provide better durability while retaining good performance.
Probing Damage in OFHC Cu Under Different Load Conditions

There has been tremendous effort to understand damage and damage evolution in OFHC Cu under high rate loading conditions. In the experiments presented in this study, a large bore gas gun was used to accelerate a flyer plate into a stationary target assembly. Photonic Doppler Velocimetry (PDV) was deployed to identify loading and unloading conditions of the target specimen. Also, with the use of a careful geometric target assembly design, soft recovery of specimen was deployed for post mortem characterization. We will present two high rate loading and unloading data sets on two specimens of OFHC Cu. Each of these specimens was subjected to two different loading paths and unloading paths, but yet each specimen was subjected to the same uni-axial tension which is known to create void nucleation. One specimen was loaded at a higher pressure in which is known to produce much more work hardening in the specimen prior to being subjected to the same uni-axial tension as the specimen loaded to a lower pressure. To try and better understand the effects of damage and damage evolution under high rate uni-axial tension, the two specimens were recovered, cross sectioned and polished to explore damage in the area under uni-axial tension. This study is an attempt to further understand and correlate high rate loading conditions to damage. We will present our findings.
Platinum (Pt) is the state-of-the-art catalyst for both anodic and cathodic reactions that occur in polymer electrolyte fuel cells (PEMFCs). Due to the cost of platinum, fuel cells have been hindered from commercialization. However, one obstacle for next generation fuel cells is to reduce the amount of platinum yet still produce tremendous activity and high durability. In this work we have investigated the effects of aging, with the use of an Accelerated Stress Test (AST) that consists of voltage cycles from 0.6 V to 1.0 V vs. RHE. Furthermore, we studied the electrochemically active surface area (ECSA) of different Pt loadings on carbon. In particular, we used a catalyst supported on a high surface area carbon, XC-72. We tested Pt catalyst of 4.8%, 20%, and 40%. These materials are used in the state-of-the-art PEMFCs. To study the activity and durability of the Pt catalyst, a rotating ring disk electrode (RRDE) system is used in stationary mode. Carbon monoxide (CO) is introduced into the RRDE system because it is adsorbed onto Pt active sites and the ECSA of the catalyst can be calculated. The number of active sites can be determined by measuring the ECSA of the hydrogen adsorption and desorption regions, and CO stripping. Detailed examination of the results reveal that the various loadings of Pt on carbon supported do have an impact on the active sites. This was validated by the decrease in ECSA as the loading of Pt on carbon increased. In all tests, we observed ECSA losses as the number of AST voltage cycles increased.

Study of Electrochemical Durability of Carbon-Supported Pt Catalysts for Fuel Cells
SEM Study of Protective Coatings Applied to Stainless Steel

There has been a great deal of research performed on erosion/wear resistant coatings for numerous applications specific to cutting and forming tools for the manufacturing, medical, aerospace and automotive industries. There exist many varieties of wear resistant coating materials and fabrication methods which are determined by specific application requirements. My research focused on selection of promising coating materials and fabrication methods for stainless steel components slated for operations under erosive and corrosive environments. I participated in fabrication of numerous coatings by physical vapor deposition (PVD), chemical vapor deposition (CVD) and chemical solution deposition (CSD) methods. In this report, I’ll present my study of the coatings microstructure and chemical composition by using scanning electron microscopy (SEM) combined with energy-dispersive X-ray spectroscopy (EDX).
Coherent Diffractive Imaging in the Near Field

Coherent diffractive imaging (CDI) is a rapidly developing form of imaging that can present substantial improvements over other types of imaging. The novelty of CDI is that lenses are not used to form an image; rather, the amplitude of the interference (or diffraction) pattern is directly imaged on a CCD, and various algorithms are used to reconstruct the phase of the sample. This is especially useful at x-ray wavelengths, where lenses are inefficient and difficult to manufacture. There are other difficulties with CDI, however. The exact relationship between light emerging from the sample (object plane) and arriving at the detector (detector plane) is nearly impossible to determine, even numerically, but becomes tractable with various assumptions. The usual set of assumptions (if the object is in the “far field”) requires the detector to be placed hundreds or thousands of meters from the sample at x-ray energies of 42 keV, which is not practical. A different set of assumptions (called the “distorted object” approach) allows imaging at any distance, but requires a balance between the detector size and distance. An indicator of this balance is a value called the “small angle number”, An, and in order that the approximation be valid, An must be much less than one. My project has been to probe where the distorted object approach fails, specifically in regards to An. Once thought to be a very stringent condition, we have found that we can obtain good quality images with An values of several thousand at visible wavelengths. This research is of interest to MaRIE project at LANL, where experiments are of necessity conducted in the near-field, and An values are virtually guaranteed to be greater than one, perhaps by orders of magnitude.
Image Based Modeling Using 3D Tomography

Through the use of image based modeling concepts alongside 3D imaging techniques, an understanding of the influence of microstructure and local damage phenomenon on the effective mechanical response of rubber-glass bead composites is sought. An emphasis is given to the microstructure-statistics-property-relations (MSPR) via an image-based (data-driven) modeling concept with incorporation of both computational and experimental protocols. Four experimental studies have been formulated to understand the effective mechanical response of these rubber-glass bead composites including: i) effect of particle volume fraction ii) local damage phenomena and it’s evolution iii) effect of particle diameter and iv) effect of surface treatments on bonding characteristics. These studies aim to capture the mechanical and morphological response of non-linear visco-elastic materials subjected to uniaxial compression. Upon collection of data and reconstruction, the microstructure-statistics-property-relations are realized through the software package, AvizoFire. Statistical characterization through this imaging software enables the formulation of MSPR. The rich data analysis collected from the various experimental studies will serve as a foundation for FEA in simulating deformation. FEA modeling of non-linear visco-elastic behavior will be conducted in the future to aid in the formulation of correlation functions at characteristic length scales and simulation of other materials of interest.
Investigation on Potting Procedures of Polyurethanes Used in Electrical Components

Electrical potting compound is one of the many applications in which polyurethanes are frequently used. This work investigated the use of polyurethanes to secure and protect nickel wires in a battery. This requires the potting material to be injected in a very small volume that is exposed to solder and solder flux during the battery’s construction. A cleaning procedure is routinely employed prior to the polyurethane potting. The objectives of the present work were the following: i) investigate the most suitable cleaning agents, ii) determine the effects of mixing procedures on the uniformity and curing of the potting, and iii) extend the pot life of the polyurethane resin. Our first experiment was to determine the best procedure to clean the flux and solder out of the battery. Solubility tests involving a series of solvents and 197 Kester flux were performed. Isopropyl alcohol exhibited the best solubility of all the solvents. Nickel wires were immersed in 197 Kester flux and cleaned by the tested solvents. The efficiency of the cleaning solvents was evaluated by NMR based on the analysis of the residues collected from the cleaned specimens. Another important goal was to evaluate procedures that could extend the polyurethane’s pot life. The common procedure only yields a usable pot life of 15 minutes. This short pot life contributes to the formation of bubbles in the final product which compromise the polyurethane’s strength. The polyurethane used in this work consists in mixing part A to part B and curing the resin at 70°C for 24 hours. The effects of mixing part A and B by hand as opposed to using a Thinky mixer were assessed. In addition, procedures involving prior heating of the starting materials were also evaluated.
Toward Stoichiometry Controlled Magneto-Transport Behavior in LaMnO3 Thin Films

We have performed a systematic study of magnetic and electronic properties of LaMnO3 (LMO) thin films produced by pulsed laser deposition. To study the effects of stoichiometry, thickness, and strain relaxation on the properties, LMO films were deposited on SrTiO3 and MgO substrates at thicknesses of 30nm, 300nm, and 1000nm. We have found that substrate and film thickness affect the magnetization of the films. The interface strain, however, is not the dominant parameter in controlling the ferromagnetic properties.
Cast duplex stainless steel piping in light water reactors experience thermal aging embrittlement during service. Interest in extending the operational life to 80 years requires an increased understanding of the microstructural evolution and corresponding changes in mechanical behavior. We are investigating the effects of thermal aging on the mechanical properties of cast CF–3 and CF–8 stainless steels using several different techniques. Tensile tests have been performed at room and operational temperatures in order to measure the bulk mechanical properties such as yield strength, ultimate tensile strength, and ductility. The results show an increase in strength and decrease in ductility after aging. Smaller length scale tests, such as instrumented nanoindentation, provide information on the local properties of the individual ferrite and austenite phases within the microstructure. Indentation results indicate an increase in nano-hardness in the ferrite phase with increasing aging temperature and time. The local phase property data can be utilized to investigate the influence of each phase on the embrittlement of the steels during aging, and can be evaluated with respect to the bulk mechanical data. This work is supported by the Nuclear Energy University Programs (NEUP), contract number DE-NE000724.
Microorganisms are critical sources for different types of bio-products including biofuels, nutrients, and drugs. Low doses of microwave radiation in the 40 - 46 GHz range have been shown to significantly enhance the growth rate of some microorganisms. Our goal for this project is to investigate the effect of high frequency microwave radiation on the growth conditions for different microorganisms. The power level and the frequency of radiation require in depth research to reproduce previous demonstrations for large scale applications. We want to identify the optimum frequency and power level that may positively influence the growth of a given microorganism. It is important to determine the propagations and penetration depths of microwave radiation through the materials of the bioreactor and the growth medium. Therefore, we first investigated microwave radiation through different materials that are typically used to make bioreactors. Next, we fabricated multiple microfluidic cells containing different thicknesses of water. The power of microwave radiation transmitted through these fluidic channels was measured using a sensor. We varied the distance of the fluidic cells from the source, the thickness of fluid, the type of fluids, and the frequency of the microwave radiation and observed how these variables affected the transmitted radiation. Our measurements showed negligible losses of microwave power while transmitting through an empty microfluidic cell. However, the transmitted power was attenuated by ten times when the thickness of the microfluidic cells filled with water increased from 50 microns to 600 microns. These findings will be utilized to design bioreactors suitable to integrate efficient microwave irradiation for growth enhancement.
Using a Film Applicator to Determine Platinum Loading for Fuel Cell Electrodes

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Moisture Sorption and Desorption of Silicone Foam

Flexible cellular silicone foams are commonly used as load-bearing materials. Therefore, the mechanical properties of the foams are fundamental for material performance. However, silicone foams are sensitive to moisture. As a result, moisture sorption and desorption of silicone foams must be characterized to better understand mechanical properties when exposed to various environments. Moisture sorption affects silicone foams by reducing the glass transition temperature. Reducing the glass transition temperature alters the mechanical properties by affecting the crystallinity of the material. In addition, moisture absorbed in the foam will slowly desorb at temperatures greater than 100°C, affecting surrounding materials. In order to study the dynamic moisture sorption and desorption of silicone foams, samples of S5470 were either dried in desiccant, or held at ambient, 50%, or 90% relative humidity. All samples were stored at 23°C. Water present in the silicone foam samples were investigated by thermogravimetric analysis, near infrared spectroscopy, and dynamic vapor sorption analysis. The experiments revealed that the foam readily absorbs moisture, but is slow to desorb moisture even at temperatures up to 200°C. Continued experiments performed on the dynamic vapor sorption analyzer will lead to kinetics mapping of water sorption and desorption in silicone foams such as S5470. Ultimately, the kinetics will be used to predict a time-moisture superposition curve. This information will lead to better understanding of the moisture sorption and desorption of silicone foams.
Efficient Curation of Heterogeneous Data Supporting Modeling of U-Nb Alloys

Given prolonged thermal aging, the properties of materials can change dramatically. Materials that are normally ductile can become brittle and strong materials can become weak. Understanding how these aging processes occur and using that knowledge to predict how the material will perform often requires analyzing heterogeneous data types (e.g., micrographs, numerical values) from many different experiments – a process that requires significant, careful data curation and can be very time consuming. In this work, we explore how one can use modern data collection, storage, and analysis technologies to accelerate the development of aging models. In particular, we have developed software to store hardness data collected for uranium-niobium alloys over 70 years of research, and use automated data analysis tools to fit models to predict how the hardness will change over time-at-temperature. We envision that the methods developed here can be used to accelerate the development of material property models for a variety of applications.
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Modelling Deformation and Recrystallization of Uranium

Modelling deformation and subsequent recrystallization of Uranium is a challenging task. We use the viscoplastic self-consistent polycrystal model (VPSC) for simulating the deformation process. In addition, for simulating heterogeneous deformation during rolling of Uranium plate we use a multiscale approach where VPSC is embedded as a user material model into a finite elements code. Material parameters are calibrated based on experimental data. Reasonable agreement of predicted and experimental stress-strain curves and textures is observed and thus it is concluded that the material model is able to satisfactorily capture the main features of the deformation process. Special attention is paid to the relationships between active slip and twinning modes and texture formation during straining. Grain reorientation trends caused by each mode of deformation are analyzed separately and in detail. Furthermore, the intragranular stress fluctuations, calculated within the deformation model, are used to calculate intragranular misorientation fluctuations. It is observed experimentally that these misorientation gradients within grains are crucial in formation of Uranium recrystallization textures. The extended model is first applied to fcc and bcc materials and results are verified by comparison with full field calculations. Finally, recrystallization is simulated using the mean field approach that includes both nucleation and grain growth. The deformation model provides the strain energy of the grains and intragranular misorientation gradients as output, both of which have been widely accepted as main parameters of the deformed state influencing subsequent recrystallization. The model is again first applied to recrystallization of fcc and bcc materials that has been studied extensively. Reasonable agreement of predicted and experimental textures is observed.
Existence of Exact Guderley Compressible Flow Solutions in Real Materials

It is known classically that in an ideal gas, there exist self-similar, spherical, converging shock solutions, but much less is understood about the existence of such solutions in compressible flow of real materials. On the other hand, it has recently been pointed out that there exist self-similar solutions for the Euler equations regardless of the equation of state closure model, which suggests the possibility that the Guderley problem might be solvable in general. In this work, we rigorously determine what properties are required of an equation of state in order for an exact, self-similar Guderley flow to be realized, including a generic solution procedure in the cases where existence holds. Among other contexts, this result is of great practical interest for the verification of codes intended to treat shock propagation in a wide variety of real materials.
Forecasting Influenza Incidence with CDC Page View Data

Influenza epidemics result in a public health and economic burden around the globe. Traditional surveillance techniques, which rely on doctor visits, provide data with a delay of 1-2 weeks. A means of obtaining real-time data and forecasting future outbreaks is desirable to provide more timely responses to influenza epidemics. We used Internet traffic data from the Centers for Disease Control and Prevention Web site (CDC.gov) to determine the potential usability of this data source. We tested the traffic generated by ten influenza-related pages in eight states within the United States and compared it against clinical surveillance data. Our results show a Pearson correlation coefficient of 0.93 in the most successful case and promising results for other cases. These results demonstrate that Internet data can complement traditional influenza surveillance, especially when there is a time lag or data is unavailable. We anticipate traffic generated from the CDC Web site may be useful for disease surveillance and informing nowcasting and forecasting models.
For many target and anomaly detection algorithms, a key step is the estimation of a centroid (relatively easy) and a covariance matrix (somewhat harder) that characterize the background clutter. For a background that can be modeled as a multivariate Gaussian, the centroid and covariance provide sufficient information for well-defined peripheral characterization. But ellipsoidal contours can characterize a much larger class of multivariate density function, and the ellipsoids that characterize the outer periphery of the distribution are most appropriate for describing the majority of the data. Traditionally the sample mean and sample covariance are used to estimate ellipsoid location and shape, but these quantities are confounded both by large lever-arm outliers and non-Gaussian distributions within the ellipsoid of interest. We aim to compare a variety of centroid and covariance estimation schemes with the aim of characterizing the periphery of the background distribution. In particular, we will consider a robust variant of the Khachiyan algorithm for minimum-volume enclosing ellipsoid. The performance of these different approaches is evaluated on multispectral and hyperspectral remote sensing imagery using coverage plots of ellipsoid volume versus false alarm rate.
A Meta-Analysis of the Association Between Gender and Health Protective Behaviors

Pandemics of respiratory diseases are unpredictable yet recurring events that levy a high cost on individuals and society. The health-protective behavioral response of the public plays an important role in limiting epidemic respiratory disease spread. Health-protective behaviors take several forms. Behaviors can be categorized as pharmaceutical (e.g., vaccination uptake, antiviral use) or non-pharmaceutical (e.g., hand washing, face mask use, avoidance of public transport). Due to the limitations of pharmaceutical interventions during epidemic influenza outbreaks, public health campaigns aimed at limiting epidemic respiratory disease spread often emphasize both non-pharmaceutical and pharmaceutical behavioral interventions. Understanding the determinants of the public’s behavioral response is crucial for devising public health campaigns, providing information to parametrize mathematical models, and ultimately limiting disease spread. While other reviews have qualitatively analyzed the body of work on demographic determinants of health-protective behavior, this meta-analysis quantitatively combines the results from 87 studies to determine the global relationship between gender and health-protective behavioral response. The results show that women in the global population are about 50% more likely than men to adopt/practice non-pharmaceutical behaviors. Conversely, men are marginally (about 12%) more likely than women to adopt/practice pharmaceutical behaviors in the general population. It is possible that factors other than pharmaceutical/non-pharmaceutical status not included in this analysis act as moderators of this relationship. These results suggest an inherent difference in how men and women respond to epidemic respiratory disease outbreaks. This information can be used to target specific groups when developing non-pharmaceutical public health campaigns and to parameterize epidemic models incorporating demographic information.
Neutral particle transport, which includes the transport of neutrons, photons, and neutrinos, is an important phenomenon in determining the behavior of nuclear reactor cores and astrophysical processes. One deterministic method of simulating the transport of neutral particles is discrete-ordinates, which involves solving the radiative transfer equation (RTE) for a finite number of discrete solid angles. Parallelization of discrete-ordinates methods for use on supercomputing clusters can be difficult, especially for 3D, unstructured, tetrahedral meshes. In this project, the weak-scaling of various parallelization schemes for 3D discrete-ordinates methods were compared using Tycho2, a discontinuous Galerkin linear elements code developed at Los Alamos National Lab. Parallelization was done in conjunction with three algorithms: a parallel sweep in the direction of transport, Parallel Block Jacobi, and a Schur-Complement parallel Krylov subspace method. All three algorithms were run on the Cray XC30 system for various numbers of energy groups, numbers of solid angles, and domain sizes. MPI and OpenMP were used to implement the parallel algorithms.
States and non-state actors seek to acquire weapons of mass destruction (WMD). In doing so they seek to acquire not only knowledge and special materials, but also special commodities that have both WMD and legitimate commercial uses, often referred to as strategic or dual-use commodities. In order to acquire these sensitive dual-use commodities, states and non-state actors must circumvent national laws implemented to comply with global agreements, treaty obligations, and United Nations resolutions. An understanding of how aspiring proliferators attempt to acquire knowledge, materials, and commodities is important to policy makers, prosecutors, investigators, and the intelligence community. We present several proliferation case studies and use this information to build a profile of techniques used by the modern proliferator, giving insight into common proliferation methods and techniques through concrete examples.
**Proliferation Case Studies: Techniques in Modern Proliferation**

States and non-state actors seek to acquire weapons of mass destruction (WMD). In doing so they seek to acquire not only knowledge and special materials, but also special commodities that have both WMD and legitimate commercial uses, often referred to as strategic or dual-use commodities. In order to acquire these sensitive dual-use commodities, states and non-state actors must circumvent national laws implemented to comply with global agreements, treaty obligations, and United Nations resolutions. An understanding of how aspiring proliferators attempt to acquire knowledge, materials, and commodities is important to policy makers, prosecutors, investigators, and the intelligence community. We present several proliferation case studies and use this information to build a profile of techniques used by the modern proliferator, giving insight into common proliferation methods and techniques through concrete examples.
Sustainability and other environmental initiatives can be a business non-starter. Though public perception of institutionalized sustainability is at a crucial and rapidly developing stage, there yet remains a perception that environmentally-oriented goals are in conflict with the institutional mission and may detract financially or temporally from achieving the mission. I argue that though the basis for sustainability goals may differ from an institution’s goals, there is a great amount of overlap between their goals as well as methodology for how these goals can be accomplished. I compare the mission and goals here at LANL to sustainability goals outlined in popular sustainability literature. I aim to explore the spaces in between these goal sets and use my work here at Los Alamos this summer as an example of how something can flourish in this space to achieve successes for LANL as an institution as well as successes for LANL’s contribution to the environment at different levels of influence. I will discuss specific projects that I have contributed to or completed this summer such as integrating sustainability initiatives into architectural specifications to “green” our construction contracts, products, and practices as well as my contribution to the LANL Smart Lab initiative to cut laboratory energy consumption by 50% in selected facilities and how both of these initiatives fill the perceived no-man’s land between successful business practices and environmental friendliness. However, institutional change does not happen overnight. These initiatives are merely examples that represent a change in corporate culture and focus to realize the commonalities between mission and environment to prove my thesis: that you really can have it all.
Pokémon Go is a new mobile game that employs the smartphone cameras and locations of players across the world as they hunt for virtual creatures and battle others in their community. With millions of players collecting image-based data for only virtual, in-game incentives throughout the world at all times of the day, this game demonstrates how New Media resources have enormous potential for aiding in IAEA safeguards, non-proliferation, and treaty verification efforts. By properly incentivizing a large number of users to actively gather data at a variety of sites and times – such as has been done for Pokémon Go – a system could gather and analyze a large amount of safeguard and verification information. In this project, we will present selected examples of crowd-based image collection efforts, virtual globes, targeted image collection, and related citizen science efforts in the context of how ‘the crowd’ could be used for safeguard data collection.
Strategy Review for the Permit Modification Request for OB/OD at LANL Facilities

Treatment of explosive hazardous waste items have presented a significant management challenge for Los Alamos National Laboratory (LANL), particularly in the light of increased regulatory scrutiny under Resource Conservation and Recovery Act (RCRA) and the hazardous waste hazardous regulations of New Mexico Environmental Department (NMED). Open burning/open detonation (OB/OD) practices are used for onsite hazardous waste treatment when an offsite facility is not a feasible option for disposal. Under New Mexico NMED these practices required ecological, human health and worker risk assessments. A permit modification request was delivered to the state for review. This presentation will examine how LANL Environmental Compliance Group work with the state of New Mexico develop the permit modification request conditions based upon risk assessment considerations for environmental and human health exposures and impacts to onsite and offsite receptors, and will discussed how this will be used to assure that the facilities stays in compliance with state and federal requirements. Also, this project will present LANL efforts for compliance and responsiveness for the facility. This project is an example of how a collaborative working relationship among permittee, their consultant and the state can starts to create a permit pathway that assure operational flexibility and mission sensitivity. Keywords: Open Burning/Open Detonation, RCRA, HWB-NMED, Risk Assessment.
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**Affordable, Configurable, Multi-Use Lab Space**

Los Alamos National Laboratory (LANL) is tasked with solving our nation’s security challenges through scientific excellence. Unfortunately, much of the lab space used for scientific research is outdated, underutilized, and not energy efficient. The current lab conditions can make it difficult for collaboration and communication among scientific teams. The goal of this project is to evaluate the benefits and costs associated with refurbishing existing lab space into a lab that can be easily reconfigured, be used by multiple disciplines, meet environmental efficiency standards, and maintain a cost effective budget. This project will address LANL’s aging lab infrastructure by providing updated, energy efficient, and flexible lab space which promotes better communication and collaboration among LANL scientists and will result in the delivery of world-class science.
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Characterization of Organically Bound Tritium in Vegetation at LANL

Tritium (3H) is used in nuclear weapons and has been processed, stored, and disposed of at Los Alamos National Laboratory (LANL). It is easily dispersible in the terrestrial environment; the rate depends on the geological and hydrological conditions and the physical form of tritium. Tritiated water (HTO) is readily incorporated into plants through root uptake and to a lesser degree from absorption through vapor exchange in foliage. The absorbed HTO follows the H2O pathways in the plant, but some of it becomes organically bound (i.e., in C-H bonds). It is important to differentiate the HTO and OBT forms since the biokinetics and internal dosimetry between tissue free water tritium (TFWT) and the organically bound tritium (OBT) for human and non-human biota are substantially different. There are only a few studies on the amount of OBT in native vegetation, and there are no comparative measurements of OBT and TFWT in native plants at LANL, which are sources of food for the local wildlife. In this study, comparisons of tritium content (total, OBT and TFWT) across three vegetation types and across the growing season were made. Vegetation samples of prevalent species in the semi-arid site were collected at the three locations near waste disposal shafts at LANL and were analyzed for tritium. The results indicated that 1) OBT is present in all species across all seasons and the levels correlate with the TFWT; 2) a buildup of OBT and TFWT from the beginning to the end of growth seasons; and 3) Juniper samples contained the highest of the TFWT and OBT among the three species suggesting greater year-round access to the higher concentrations of HTO hypothesized to be located within deeper soils.
Waste Compliance and Tracking System Recommendations for Higher Quality WSP

To ensure success and compliance with legal mandates and requirements, the software application Waste Compliance and Tracking System (WCATS) supports the generation, characterization, processing, shipment and receiving of all waste types at the Los Alamos National Laboratory. WCATS Waste Stream Profiles (WSPs) capture waste characterization descriptions to ensure waste is managed, stored and treated safely and properly from cradle-to-grave. WCATS currently has criteria and validation checks resulting in warnings or errors in WSPs to signal weak characterization documentation. This project is about recommending new criteria to implement for the software program to further enhance expectations, combat profile deficiencies, and produce accurate, sufficient and up-to-date WSPs. The new criteria will contribute to optimizing compliance, reducing hazards and improving safety associated with waste processing and management. These recommendations will impact the number of warnings and errors causing them to temporarily increase in the WCATS system. This poster addresses the recommendations of new criteria to be evaluated.
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Quantum Effects in Free Electron Lasers

Free electron lasers (FELs) are unique sources of intense short wavelength radiation. In FEL, relativistic electrons moving in a periodic magnetic field form microbunches that coherently emit light. In X-ray regime, FEL typically starts from noise. This regime is called self-amplified spontaneous emission (SASE). In this contribution, we analyze the influence of quantum effects on FEL performance. Namely, we treat every electron as a wavepacket, rather than a point particle. It allows us to properly analyze start up of SASE FEL from noise and estimate the role of finite size of electron wavepacket for it. We also numerically study one-dimensional SASE FEL within semi-classical framework and compare results with predictions of classical theory. The limits of applicability of classical theory as well as simplified description of all electrons with one wavefunction are found. Finally, we apply this approach to the planned MaRIE FEL and show how quantum effects can affect its performance.
The effects of Reynolds (Re) and Atwood (A) numbers on turbulent mixing of a heterogeneous mixture of two incompressible, miscible fluids with different densities are investigated by using high-resolution Direct Numerical Simulations (DNS). In a triply periodic domain, the two fluids are initially segregated in random patches and the mixing occurs in response to stirring induced by buoyancy-generated motions. Statistically homogeneous variable-density (VD) mixing, with density variations due to compositional changes, is a basic mixing problem and aims to mimic the core of the mixing layer of acceleration driven Rayleigh-Taylor Instability (RTI). In this study, results are covering a large range of kinematic viscosity values and density ratios including small (A=0.05), moderate (A=0.25 and 0.5), and high (A=0.75) Atwood numbers. The structure of the flow is investigated by decomposing the flow into the different flow regions by the density value. It is shown that the divergence of the Lamb vector, which identifies inhomogeneities in the momentum transport surrounding a fluid element, is mostly negative in lighter fluid regions and mostly positive in heavier fluid regions. This indicates that the turbulence is mainly generated in light fluid regions; in contrast, the heavy fluid regions act as a kinetic energy storage mechanism. Fundamental differences are also detected between the light and heavy fluid regions, especially at higher A values, in terms of the structure of turbulence, flow evolution and alignment between various turbulence and scalar quantities. The results point to a much more complex picture of the flow than the current models suggest and the need to update these models.
Progress Towards a Potassium BEC Machine

The Quantum Technologies group at Los Alamos National Laboratory uses Bose-Einstein Condensate (BEC) matter waves and a “Painted Potential” laser system to create ultrasensitive rotation and acceleration sensing technology. The current experimental setup uses a BEC made of 87-rubidium atoms, but interatomic scattering forces can cause the matter waves to lose coherence during an experiment. Our group is building a new experimental setup that uses 39-potassium atoms instead, which have the advantage that these scattering forces can be tuned to nearly zero. The setup consists of two Magneto-Optical Traps (MOTs), an optical dipole trap transport system, and a glass cell where the BEC will encounter the Painted Potential. We describe our progress towards building the described setup and tuning our experiment, with the goal of creating a potassium BEC.
EOSlib: Cross-Platform Build and Test

Abstract. EOSlib is an equation of state library and database program created at Los Alamos National Labs by Ralph Menikoff. The software has the ability to fetch material parameters, change units, evaluate thermodynamic quantities for numerous EOS fitting forms, calculate shock isentrope and isotherm loci for an inert, detonation and deflagration loci for an explosive and solve Riemann problems for two materials with different EOS's. The program's extensive capabilities have been greatly limited, however, by its platform dependency. A platform independent build, compile and test process will greatly increase this software's usability. This process is provided through CMake, an open-source make system used to control the software build and compile process. The testing is provided through CTest, a software utility included within CMake, which can be configured to automate the testing process. Through the use of this make system, EOSlib source files can be automatically installed and tested on multiple platforms, eliminating a large barrier to the software's increased implementation.
Muon Detector Fabrication for Structural Analysis of the Santa Maria 'Cupola'

The Santa Maria del Fiore Dome and Muon Imaging  The dome of the Cathedral of Santa Maria del Fiore, built without temporary supports by Filippo Brunelleschi in the 15th Century, has led scholars to question whether there are supports in the internal makeup. Cracking in the dome over the centuries has created a necessity for detailed knowledge of the interior structure to aid in evaluations of static and dynamic (earthquake) conditions. Muons, a highly penetrative subatomic particle, have the ability to discriminate between materials of different atomic (Z) number based on scattering interactions. Radiography with cosmic ray muons is being explored as a technology to determine the internal structure of the dome walls. The cramped spaces inside the dome call for a modular muon detector that can be assembled on site. Two 1.2m x 1.2m drift tube detectors, each made of small modules, are being constructed to be used to image the dome substructure. The construction of these detector modules consisted of cleaning and assembling parts, leak testing evacuated systems, and checking electrical signals so the final detector assembly is able to detect any reinforcements inside the dome of the cathedral.
The dome of the Cathedral of Santa Maria del Fiore, built without temporary supports by Filippo Brunelleschi in the 15th Century, has led scholars to question whether there are supports in the internal makeup. Cracking in the dome over the centuries has created a necessity for detailed knowledge of the interior structure to aid in evaluations of static and dynamic (earthquake) conditions. Muons, a highly penetrative subatomic particle, have the ability to discriminate between materials of different atomic (Z) number based on scattering interactions. Radiography with cosmic ray muons is being explored as a technology to determine the internal structure of the dome walls. The cramped spaces inside the dome call for a modular muon detector that can be assembled on site. Two 1.2m x 1.2m drift tube detectors, each made of small modules, are being constructed to be used to image the dome substructure. The construction of these detector modules consisted of cleaning and assembling parts, leak testing evacuated systems, and checking electrical signals so the final detector assembly is able to detect any reinforcements inside the dome of the cathedral.
Benchmarking of Vector Particle-In-Cell (VPIC)
Binary Collision Model in Dense, Gas-M

Collisional relaxation rates for ion and electron plasma test particles in a variety of background plasma media have been evaluated through a series of Vector Particle-In-Cell (VPIC) simulations on the LANL Mustang supercomputer. These calculations apply a non-relativistic, binary collision operator to model small-angle, inter-particle scattering processes. In these simulations, comparisons have been made between simulated and theoretical stopping, perpendicular scattering, and parallel scattering (i.e., straggling) rates. These comparisons have been performed at various beam speeds and the sensitivity to background particle sort frequency has been examined. Generally, good agreement is observed between simulated and theoretical relaxation rates and this study provides necessary guidance for what particle sort frequencies are appropriate for different test particle beam speeds. If time permits, a similar evaluation of a relativistic scattering operator will be presented.
Domain Partitioning and Problem Space Representations for Compact Binary Mergers

With the recent groundbreaking discovery of gravitational waves from merging black holes, the first direct detection of neutron star mergers is only a matter of time. Observational signatures include gravitational waves and faint supernova-like transients powered by radioactive decay of freshly synthesized heavy elements. Due to the complexity of the problem, the only way to understand these observations is to confront them with the predictions obtained via simulation. We use smoothed particle hydrodynamics, which is well suited for such problems, and adapt the highly scalable 2HOT code to simulate these mergers. Furthermore, we augment 2HOT by incorporating tabulated equations of state to improve the physics accuracy. This new physics introduces overhead. Retaining performance while adding new physics provides a unique opportunity to exercise the principles of co-design and for a collaboration between domain and computer scientists. To maintain performance and scalability, we explore and optimize the nearest-neighbor search algorithm intrinsic to the code. We develop a custom k-nearest neighbor proxy application, which provides the platform upon which we experiment with different domain partitioning schemes and problem space representations. To understand and optimize load-balancing, we also investigate implementations of our proxy application in various task-based runtime systems such as Charm++ and STAPL.
Dalton's Law and Amagat's Law were developed in order to describe the behaviors and properties of mixtures of ideal gases. These mixture rules are being used today to describe the equation of state of several multi-component materials. These materials are generally in the high energy density or warm dense matter regime. There exists little data about certain metal mixtures when they are at pressure of above 10 megabars. The predictions offered by Dalton's Law and Amagat’s Law show increasing disagreement for NiAl mixtures that we study here. Recently fielded experiments focused on the equations of state for nickel, aluminum (Swift, Paisley, McClellan, Ackland, 2007), and a nickel/aluminum alloy. A ramp pulse from the Omega-EP laser lasting four nanoseconds provides a shock that allows us to determine the properties of these materials and their alloys, and the RAGE code is being used to model the experiments. These tools should allow us to discern whether Dalton's Law or Amagat's Law is more useful for the predictions of NiAl alloy equations of state behavior in the warm dense matter regime.
High Pressure Physics with Diamond Anvil Cells

The Shock and Detonation Physics Group (M-9) supports LANL’s stockpile stewardship mission with highest quality static and dynamic equation of state (EoS) data alongside advancements in related technological capabilities. With diamond anvil cells (DAC), materials are analyzed under high-pressure and high-temperature conditions to extract fundamental data such as phase boundaries, structural changes, and material strength. Working with M-9 has introduced me to static high pressure research with DAC designs in SolidWorks, x-ray diffraction (XRD) experiments at Advanced Photon Source at Argonne National Laboratory (ANL), and extensive diffraction spectra analysis, including development of custom analysis algorithms. Various projects from the past year are presented including: (1) Livermore Style and EasyLab DAC models, (2) large volume Paris-Edinburgh press experiments and measurement capabilities, and (3) data analysis techniques including methods for peak detection, baseline creation and false peak removal.
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EOSlib: Interactive Manual

Equations of state are a vital part of scientific computing, but the process of implementing them can be both complex and error-prone. EOSlib is a software library of equations of state written by Ralph Menikoff. This library includes the Ideal Gas, JWL, and Davis EOSes that can be used to solve a variety of burn-related thermodynamic problems. Included in this library are also a set of driver scripts that apply the equations of state to specific problems. As an example, one script uses those equations to model the ZND profile of a detonation wave as it propagates through a material. Users can access an interactive manual for complete descriptions and instructions on running the utility codes with set boundary conditions. The manual exists as a set of Python notebooks that contain executable examples. These give the user a feel for how and when to apply the codes. A general index with short overviews of the utility codes is included, along with more in depth pages for each code's application peculiarities. The library and the manual are available on LANL HPCs.
In this project we modeled a component of pulsar wind nebulae (PWNe), a supernova remnant where the star’s core has collapsed into a pulsar. Pulsars are neutron stars that possess magnetic fields misaligned with their axes of rotation along which particles are accelerated to relativistic speeds. The “pulse” they give comes from this beam of charged particles periodically turning towards the earth. Within a PWN, the pulsar’s stream of charged particles pushes on the matter of the supernova remnant, creating the expanding, shocked nebula. We are studying the pulsar bubble, a region between the pulsar and the ejected matter that is filled with a turbulent magnetic field. Here, the motion of particles can be well modeled by diffusion, but the transport coefficients are unknown. In order to determine these coefficients, we used a Monte Carlo code that tracks individual particles moving over a large sample of turbulent fields constructed by superimposing randomly oriented Alfvén waves. Analyzing these simulations we can extract transport coefficients, such as diffusion coefficients and advection velocities allowing us to investigate the impact of various parameters which change the character of the diffusion. The important factors for us to understand are related to the structure and spectrum of the turbulent field and the distribution of the particles. In investigating how these parameters impact the diffusion of the particles, we hope to find the diffusion coefficients so that they can be used in later models of PWNe.

**Turbulent Magnetic Field Sampling for Pulsar Wind Nebulae**
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Verification problems test a computer code’s ability to numerically solve a problem with a known exact solution. This is useful because by correctly solving a problem with a known solution, it increases our confidence that it can solve more complex problems for which the solutions are unknown. Here we revisit the Noh verification test problem. The one-dimensional planar Noh problem is comprised of a compressible, ideal gas of negligible viscosity that is initialized with a uniform, inward velocity, impinging on a hard wall. This flow pattern creates an outgoing shock wave at the origin, and is commonly used to assess a code’s ability to convert kinetic energy into internal energy. These characteristics of the Noh problem make it simple, yet difficult for most hydrocodes to properly simulate. Traditionally, the Noh problem is run using an ideal gas. Recently, however, Burnett et al, have shown that an analytical solution may also be obtained with the “stiff gas” equation of state. The stiff gas is relatively simple in form but gives a qualitatively accurate representation of many metals, while allowing condensed-phase materials to go both into compression and tension. Here we implement the stiff-gas EOS in the Noh problem to model the behavior of aluminum, copper, iron and tungsten under shocked or extreme conditions and evaluate the code’s ability to follow the thermodynamic behavior of the material. These hydrodynamic verification studies were done using the LANL Eulerian code xRAGE and the LANL Lagrangian code FLAG. Numerical results are compared to the exact stiff-gas results and to the experimental shock Hugoniot, and mesh convergence studies are performed. Our results show that this classic and widely-studied verification test problem can be extended beyond the ideal gas to physically realistic materials of practical interest.
Characterizing Magnetic Rayleigh-Taylor Instabilities using 2D Lagrangian RMHD Code

Magnetically driven implosion experiments are a proven method of developing high-energy shock experiments on microsecond timescales. By applying a large (10-100 MA) current pulse through a thin aluminum cylinder, a large magnetic pressure due to the Lorentz force causes the thin walled liner to implode without the use of high explosives. These liner implosion experiments are a proposed method for the shock generation of warm dense matter (WDM)[1][2], a very high density plasma found in solar and planetary cores. Ohmic heating due to resistive diffusion typically causes melting of the liner. This melted region is then subject to magnetic Rayleigh-Taylor (mRT) instabilities which reduce the liner performance the transfer of energy into the target. In order to reduce the effects of Ohmic heating and allow higher current drivers, a Kick-and-Coast method is proposed[3]. This method would increase the radius of the liner thus reducing the current density while increasing the timescale of the implosion past that of the current pulse. This gives an initial "kick" to the liner after which the cylinder ceases to accelerate in its center of mass reference frame. Due to the incompressible nature of the liner, the inner surface of the cylinder experiences a final acceleration as the liner thickens just prior to impact. To maximize the proposed benefits of the Kick-and-Coast method, RAVEN, a 1D magnetohydrodynamic (MHD) code was used to determine optimal liner radius and thickness based off maximum velocity and kinetic energy at impact with minimal acceptable melting (~50%). Three optimal sizes of liner were then tested for RT instabilities using a 2D MHD code called FLAG. The resulting liner implosion performance demonstrated the degree of viability of the Kick-and-Coast setup for shock generation of WDM.
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Aneurysm Physics Can be Lethal

The human circulatory system consists of vessels that transport blood throughout the body, providing the tissues with oxygen and nutrients. An aneurysm is a localized enlargement of an artery caused by a weakening of the artery wall leading to rupture and possible death. When an aneurysm forms there are no symptoms to be felt, the symptoms only appear after the aneurysm has ruptured. When the aneurysm ruptures internal hemorrhaging occurs which can be fatal. We carried out simulations to test the hypothesis that sensitivity of aneurysm formation depends on vessel wall rigidness and other variables. We present simulation results and possible implications.
Infrared Spectra of Ammonium Nitrate at Hydrostatic Pressures up to ~20 GPa

High pressure-temperature (P-T) studies of material properties are important in order to develop accurate equation of state models and for improving our ability to model the response of materials under extreme conditions. Ammonium nitrate (AN) is a widely used chemical, most commonly used as fertilizer, but more relevant to LANL it is also an explosive. While it is known that AN changes structural phase depending on temperature, phase changes based on high pressure have been less investigated. Diamond anvil cell techniques were applied in experiments, which were designed to characterize the phase stabilities of AN at high pressures and room temperature. Using the infrared beam line at the National Synchrotron Light Source (NSLS), two duplicate high pressure experiments were performed at room temperature, in which the pressure was increased in intervals of approximately 1 gigapascal (GPa) to a final pressure of 20 GPa. Infrared (IR) spectroscopy was performed on the samples contained in the diamond anvil cell, while standard ruby fluorescence technique was used for determining changes in pressure. By observing the shifts in the IR active vibrational modes, structural stability can be linked to molecular structure. While we observed shifts in the known phase IV peaks, there were no changes in the spectrum that would be associated with a phase transition. It was concluded that no phase transition occurred with the increase in pressure, and AN remained in the stable phase IV throughout the process. While this research contributes to validating the current equation of state, continuing to explore the stability of AN at high temperatures and pressures is critical to understanding the behavior of AN as an explosive and for other applications.
In this work we will report the fabrication of monodispersed alginate microspheres using droplet based microfluidics. Droplet based microfluidics is one of the most efficient methods to create monodispersed aqueous droplets in an oil. However, critical challenges exist in integrating the typical gelation chemistry of alginate formation into a microfluidic platform: if the alginate crosslinks too quickly it may clog the microfluidic channels, whereas if the crosslinking is too slow, the droplets formed may clot to form one large cluster. Therefore, we will optimize a delayed gelation chemistry of alginate hydrogels for integration into the microfluidic format. The droplet generator in our lab is a small microfluidic chip. It uses a combination of 4 inlets. The inlets are arranged such the alginate and calcium solutions combine through a Y junction that eventually leads to a T junction where the two streams of oil meet. The mixture is pinched off, forming droplets in a continuous fashion. Following the droplet generation, the alginate beads will be characterized for shape and size distribution using microscopy. These mono-dispersed alginate based microspheres can be used in many applications as cell cultures, injectable cell carriers, etc.
**Domain Partitioning and Problem Space Representations for Compact Binary Mergers**

With the recent groundbreaking discovery of gravitational waves from merging black holes, the first direct detection of neutron star mergers is only a matter of time. Observational signatures include gravitational waves and faint supernova-like transients powered by radioactive decay of freshly synthesized heavy elements. Due to the complexity of the problem, the only way to understand these observations is to confront them with the predictions obtained via simulation. We use smoothed particle hydrodynamics, which is well suited for such problems, and adapt the highly scalable 2HOT code to simulate these mergers. Furthermore, we augment 2HOT by incorporating tabulated equations of state to improve the physics accuracy. This new physics introduces overhead. Retaining performance while adding new physics provides a unique opportunity to exercise the principles of co-design and for a collaboration between domain and computer scientists. To maintain performance and scalability, we explore and optimize the nearest-neighbor search algorithm intrinsic to the code. We develop a custom k-nearest neighbor proxy application, which provides the platform upon which we experiment with different domain partitioning schemes and problem space representations. To understand and optimize load-balancing, we also investigate implementations of our proxy application in various task-based runtime systems such as Charm++ and STAPL.
Modeling of Layered Atmospheres in X-Ray Bursting Neutron Stars

The accretion of material onto an X-ray bursting neutron star (XRB) results in a bright, thermonuclear reaction that consumes the accreted matter. From this reaction, the atmosphere glows in X-rays for a few seconds, which allows for observations of the atmosphere's spectra. Simulated spectra can be compared to observational measurements from X-ray telescopes; in comparing the simulations and observations, we can probe the mass and radius of the neutron star. Current simulations use a uniform-atmosphere approximation to model these spectra. But, like all realistic spectra, the simulated spectra are strongly dependent on atmospheric composition. The composition, which is typically mixed, then has a significant impact on the shape and energetics of the spectra. So, in making the approximation of a uniform atmosphere, these models neglect the impact of the mixed atmospheric compositions on the XRB spectra. We present results on the evolution of these models to a layered atmosphere, which is the first step in simulation of processes that contribute to the non-uniformity of the atmosphere's composition—like accretion, mixing, and mass loss. To model atmospheres with layered compositions, we have added features to Zcode—a radiative transfer code developed at Los Alamos National Laboratory—to model XRB atmospheres with homogeneous compositions. In conducting the layered simulations, we found that there was a significant difference from the spectra of uniformly composed atmospheres. In addition to the spectral differences, the atmospheric temperatures and densities had distinctly different profiles, further indicating the importance of non-homogeneous compositions in this problem. From our results, we have begun developing more realistic models to compare with physical observations; our next step is to model composition gradients due to atmospheric mixing processes.
Gas gun experiments have the potential to investigate material properties in various well defined shock conditions, making them a valuable research tool for the development of equations of state (EOS) and material response under shock loading. Gas guns have the ability to create shocks for loading to pressures ranging from MPa to GPa. A variety of diagnostics techniques can be used to gather data from gas gun experiments; resulting data from these experiments is applicable to many fields of study. The focus of this set of experiments is the development of data on the Hugoniot for the overdriven products EOS of PBX 9501 to extend data from which current computational EOS models draw. This series of shots was conducted by M-9 using the two-stage gas-guns at LANL and aimed to gather data within the 30-120 GPa pressure regime. The experiment was replicated using FLAG, a Lagrangian multiphysics code, using a one-dimensional setup which employs the Wescott Stewart Davis (WSD) reactive burn model. Prior to this series, data did not extend into this higher range, so the new data allowed for the model to be re-evaluated. A comparison of the results to the experimental data reveals that the model is a good fit to the data below 40 GPa. However, the model did not fall within the error bars for pressures above this region. This is an indication that the material models or burn model could be modified to better match the data.
Plasma modeling can be conducted with varying levels of detail. The Bhatnagar-Gross-Krook approximation is an effective kinetic model for hot plasma given an accurate relaxation parameter. This parameter, however, is difficult to know a priori. Molecular dynamics offers a fully detailed model for ionic motion. The heterogeneous multiscale method (HMM) provides a computational and analytical link between disparate physical models. In this paper, we present a proof of concept of HMM as a modeling method for hot plasma. The unknown relaxation parameter can be computed from short molecular simulations, and then used in subsequent kinetic time steps. Simulations using the hybrid kinetic-molecular dynamic model are both more accurate than the kinetic model alone, and orders of magnitude more efficient than the molecular dynamics model alone. The HMM philosophy can be used similarly to hybridize physical models in a way that creates a stark improvement over both original models.
Ultra cold neutrons (UCN), or neutrons with a velocity less than 7 m/s, likely hold the answers to several fundamental questions such as why matter dominates over antimatter in our universe and how the lightest elements were created directly after the Big Bang. One of the key limiting factors in all UCN experiments is the number of UCN available. Los Alamos Neutron Science Center (LANSCE) still houses one of the world’s most intense UCN sources, which can be improved further, if we can, for example, reduce the para-deuterium fraction in the deuterium ice used to make UCN. Raman spectroscopy is a sensitive probe that has been used for the UCN source improvement. We show that the existing experimental setup and data analysis yield a para-sensitivity of more than 10 percent. A new cosmic-ray background reduction algorithm improves the sensitivity to a few percent. A survey of other techniques is given and compared, with a goal to reach a para-fraction sensitivity of 0.1% in the near future.
Due to a combination of tradition and HE product confinement issues, the majority of simple explosive tests at LANL have been based on a cylindrical design. However, a flat, sandwich-like setup offers quite a few advantages over the traditional geometry, including less costly machining and a more focused and accurate analysis of explosive equations of state. Over the course of a year, we designed and modeled a series of “sandwich” tests in the ASC hydrocode FLAG. This work culminated in the fabrication and testing of several of the model designs at the Chamber 8 enclosed firing facility. The experimental series consists of three separate shots with a similar setup-- two of them using copper confinement and one confined by tantalum. At the moment, only the tantalum shot has been fired, so this work focuses on that shot. The shot was driven by a 130 mm by 150 mm PBX 9501* slab with a uniform thickness of 10 mm. The slab was sandwiched on either side by two 130 mm by 150 mm sheets of Tantalum with a nominal thickness of 0.55 mm. These detonating explosives accelerated the metal confinement into a volume held at vacuum. The time-dependent velocity of the metal plates were measured by four PDV** probes aligned normal to the surface of the sandwich. This poster presents a comparison of the predicted metal velocities to the measured metal velocities and discusses post-shot modifications of the model necessary to produce better matches to the experimental data. * PBX-9501 is a type of polymer-bonded explosive consisting of 95% HMX and 5% binder ** PDV, standing for Photon Doppler Velocimetry, is a method for measuring velocity using laser interferometry.
Gas Cherenkov detectors (GCD) produce Cherenkov light when relativistic electrons enter the gas filled detector volume moving faster than the local allowed speed of light. In order to slow down, these electrons emit energy in the form of Cherenkov light. GCD are an enticing option for use in inertial confinement fusion systems due to their fast timing resolution (~10ps). While GCD are capable of measuring at ultra-short timescales, these detectors are limited by photomultiplier tube (PMT) technology which typically has a time resolution of ~100ps. In order to take advantage of the fast time resolution of GCD, pulse dilation was used to increase the timing resolution of a microchannel plate photomultiplier tube (MCP-PMT). Pulse dilation is a technique where the signal from a PMT is manually stretched (20x) in time allowing for better resolution. The signal is then recompressed during post processing. The signal is dilated by adding a mesh with a time varying voltage potential between the photocathode and anode. The voltage potential causes the electrons to accelerate at different rates based on when an electron was created. A time separation is created by drifting this electron signal for a short distance before measurement. The result is an output signal stretched in time from the MCP-PMT with ~10ps timing resolution.
The Gruneisen equation of state is an analytic equation of state designed to model materials whose atoms are restricted to small vibrations, such as in crystalline solids. Analytic equations of state are desirable when finding exact solutions to hydrodynamics code verification problems such as the Noh, Sedov, and Guderley test problems. These problems are self similar. In the general case the Gruneisen EOS is not compatible with hydrodynamic scaling phenomena, however, it does exhibit scaling behavior in the special case of the one dimensional planar Noh problem as discussed by Ramsey, Boyd, and Burnett. This discourse explores the compatibility of this scalable form of the Gruneisen EOS with the Lagrangian multi-physics code, FLAG, over a wide range of material parameters. A mesh convergence study examines the simulation discretization errors associated with extreme materials for this analytic equation of state.
Optical coherence tomography (OCT) has many potential applications in microfluidics. We have investigated several applications including surface profiling, determination of particle velocity, and quality control of microfluidic devices, using an off the shelf OCT platform from Thorlabs. Thin and flexible membranes integrated into microfluidic devices were characterized for their flatness using 3D confocal imaging, and compared to 3D OCT. Velocity profiles in the microfluidic channels were characterized using 40 micron particles at ~10 microliters per minute flow rates. Quality control of rapidly prototyped multiple microfluidic devices were carried out using fast volume rendering mode of the OCT platform. These are just three of an expanding list of application that OCT could potentially be used in microfluidics.
With the recent groundbreaking discovery of gravitational waves from merging black holes, the first direct detection of neutron star mergers is only a matter of time. Observational signatures include gravitational waves and faint supernova-like transients powered by radioactive decay of freshly synthesized heavy elements. Due to the complexity of the problem, the only way to understand these observations is to confront them with the predictions obtained via simulation. We use smoothed particle hydrodynamics, which is well suited for such problems, and adapt the highly scalable 2HOT code to simulate these mergers. Furthermore, we augment 2HOT by incorporating tabulated equations of state to improve the physics accuracy. This new physics introduces overhead. Retaining performance while adding new physics provides a unique opportunity to exercise the principles of co-design and for a collaboration between domain and computer scientists. To maintain performance and scalability, we explore and optimize the nearest-neighbor search algorithm intrinsic to the code. We develop a custom k-nearest neighbor proxy application, which provides the platform upon which we experiment with different domain partitioning schemes and problem space representations. To understand and optimize load-balancing, we also investigate implementations of our proxy application in various task-based runtime systems such as Charm++ and STAPL.
A Heterogeneous Multiscale Model for Plasma Simulation

Plasma modeling can be conducted with varying levels of detail. The Bhatnagar-Gross-Krook approximation is an effective kinetic model for hot plasma given an accurate relaxation parameter. This parameter, however, is difficult to know a priori. Molecular dynamics offers a fully detailed model for ionic motion. The heterogeneous multiscale method (HMM) provides a computational and analytical link between disparate physical models. In this paper, we present a proof of concept of HMM as a modeling method for hot plasma. The unknown relaxation parameter can be computed from short molecular simulations, and then used in subsequent kinetic time steps. Simulations using the hybrid kinetic-molecular dynamic model are both more accurate than the kinetic model alone, and orders of magnitude more efficient than the molecular dynamics model alone. The HMM philosophy can be used similarly to hybridize physical models in a way that creates a stark improvement over both original models.
Ptychography is a two and three-dimensional imaging technique developed as a means of improving diffraction microscopy techniques and addressing the phase retrieval problem through providing additional support in the form of redundant diffraction information. We report on imaging and reconstruction techniques utilizing the Relaxed Averaged Alternating Reflection algorithm for data taken on a high harmonic tabletop source and at the LINAC Coherent Light Source on various micron and submicron test patterns. Utilization of additional diffraction support for improving reconstructions is demonstrated. Exploit of this technique for imaging magnetic domain structure in antiferromagnetic and ferromagnetic materials at soft X-Ray wavelengths is discussed.
Nucleation is the process by which a metastable phase decays into a stable phase. It is widely observed in nature, and is responsible for many phenomena like cloud formation and crystal growth. The classical nucleation theory predicts a compact droplet of the stable phase that will initiate the nucleation process. For many systems with long range interactions, however, the droplets are highly ramified and harder to locate due to lack of a well-defined structure. I have been studying nucleation in Lennard-Jones liquids, by performing Molecular Dynamics simulations in a Micro-Canonical ensemble of Argon particles. The system is quenched from liquid temperatures into a metastable solid phase, and allowed to evolve under constant energy dynamics. I investigate the symmetry of the critical nucleus by pinpointing its exact location and time of appearance and employing spherical harmonics to identify the spatial arrangement of molecules. The deeply quenched region far from coexistence exhibits non-compact droplets with structures far removed from the stable fcc phase. This could be an indicator of spinodal nucleation, giving us an idea of the limit of metastability (pseudospinodal).
Assessing Modulated-Laser PDV

Photon Doppler velocimetry (PDV) is a secondary diagnostic used in Proton Radiography at Los Alamos National Laboratory. PDV measures the velocity of a moving surface by detecting the beat frequency between the unshifted and Doppler-shifted laser light. Typically, the digitizers used to record PDV signals are very costly. The goal for this project is to reduce the digitizer bandwidth requirements. One way to lower the cost of PDV is to reduce the frequency of the PDV signal. This can be done by modulating the laser. The modulated-laser PDV experiment was successfully done. And the results are consistent with the theoretical predictions and previously published work. This will enable surface velocimetry with greatly reduced digitizer bandwidth requirements.
The B-61 Life Extension Project is important to maintain the safety and quality of the United States Nuclear Stockpile. A required component of stockpile stewardship is being able to accurately predict the behavior of the explosive PBX 9502. This explosive, a composite of TATB and Kel-F 800, is very insensitive. The experiments done in 2001 by Richard L Gustavsen (M-9) form much of the basis for the current model used for the response of PBX 9502 to shock. This calibration data is based on high quality 1-D impacts. This series of gun experiments helps to prove the validity of the current working model for both 1 and 2-D shocks. The current explosive reactive burn model (SURF) is based off a distinctive shock wave form in which the rear shock release is the defining component of shock attenuation. However, in a 2-D space, the waveform is more complex. The object of this experimental series is to determine whether the existing model can correctly predict explosive response to both 1-D and 2-D shock data. The 1-D experimental series is conducted by shooting a thin sheet of stainless steel (with the aid of a polycarbonate sabot) at a sample of PBX 9502. The 2-D shock setup uses a dense metal rod inserted into the front face of a polycarbonate sabot as a projectile, aimed at sample of PBX 9502. In both experimental setups, the velocity of projectile is measured with a magneto-electric speed device, and the projectile’s impact and HE response is then captured with high speed and framing cameras. This data is then compared against the model for fit. The expectation is that the SURF model will more accurately predict the 1-D shock insults, and it will be determined if the SURF model possesses the same predictive power in regards to the 2-D shock insults.