POSTER PRESENTATION ABSTRACTS

SYMPOSIUM 2007

BIOSCIENCE

Ethan Brown
University of Oklahoma
P-21
Garrett Kenyon

Presentation Title: Invariant Feature Recognition Using Dendritic Processing

Presentation Abstract: The fundamental building blocks of the mammalian visual system are cortical edge detectors--simple cells in V1 that respond selectively to short lines segments of a preferred orientation. Hubel and Wiesel proposed that these cells receive their input from optimally aligned sets of LGN relay neurons. However, current feed-forward models of layer 4 visual cortex simple cell edge detectors fail to account for the experimentally measured low aspect ratio (between 1:1 to 2:1) of the input LGN receptive fields. We hypothesize that nonlinear dendritic subunits of higher aspect ratio could enable good orientation selectivity for V1 simple cells despite the low aspect ratio of their retinotopic input. First with passive dendritic structure at high aspect ratio, we confirm our model reproduces those results present in current experimental results, i.e. orientation tuning, contrast invariance, spatial frequency tuning, and weak small spot responses. Next, we show at low aspect ratios, passive dendritic structure is incapable of reproducing the measure response properties of V1 simple cells. Finally, we initialize dendritic spiking through nonlinear subunits in order to once again regain the experimentally observed behavior. Furthermore, nonlinear dendritic subunits could provide a general mechanism whereby neurons in higher visual areas acquire selective responses to very specific features regardless of scale, translation, or rotation. In all modeling, we utilize the NEURON environment to simulate a biophysical model of V1 layer 4 simple cells.

Shannon DeAguero
NNMC
B-2
Mentor: Anu Chaudhary

Presentation Title: Examining the role of intracellular tyrosine residues in TLR4 signaling

Presentation Abstract: Toll-like receptor 4 (TLR4) is a transmembrane protein on the surface of the cell which binds to a specific prime component in microbes of gramnegative bacteria called LPS (lipopolysacchride). Innate immune response is believed to be one of the most ancient forms of protection generated by our immune system against pathogens, the toll like receptors are a key component of this reaction. When any given microbe penetrates the surface barriers (anatomic barriers such as skin and mucous membranes, or physiologic barriers such as body temperature and pH levels) toll like receptors on cells recognize various components of microbes leading to the intracellular changes that ultimately result in cytokine release. This release is the primary action which triggers an immune cell response. We have previously shown that TLR4 gets tyrosine phosphorylated upon LPS engagement. This means that the residue of the amino acid tyrosine on the surface of the receptor expresses proteins which bind to a phosphate group and switch the enzymes “on”. We have also shown association of TLR4 with tyrosine kinase Syk in THP-1 cells (Chaudhary, Fresquez, Naranjo, Immunology and Cell Biology 2007). We are interested in identifying tyrosine residues that play a role in TLR4 tyr phosphorylation upon LPS engagement. Additionally, we want to investigate the role of these residues in LPS mediated cytokine release. We employ THP-1 cells, a human monocytic cell line, in this study. LPS stimulation of THP-1 cells that have not been treated or that have been transfected with wild type TLR4 DNA or mutated TLR4 DNA where the amino acid tyrosine has been exchanged to alanine at four different positions will allow us to assess the role of tyrosines in early TLR4 signaling.

Nathan Duval
Adams State College
D-3
Mentor: Cathy Cleland

Presentation Title: Stability of Diverse Pathogens in Indoor Environments

Presentation Abstract: Following a bioterrorist incident in an indoor environment (e.g., the October 2001 Hart Senate Office Building anthrax attack) air and surface samples may provide significant information that would facilitate the remediation process. Sampling would enable efficient and effective decontamination by allowing for quick identification of the contaminant, assessing the extent of contamination, and monitoring of the remediation process. Expeditious remediation efforts are crucial to ensure public safety and lessen the economic impact. Sampling in an indoor environment presents many difficulties given the variance of the surfaces, the isolated areas where agents can accumulate and thrive, and the possibility of secondary aerosolization. To ensure an immediate and cost-effective decontamination capability, we must first understand the fundamental characteristics of the potential agents. These characteristics include persistence on indoor surfaces, decay rates, and resistances or susceptibilities to decontamination strategies. Secondly, the characteristics of the indoor environments must be understood, this includes the porosity of surfaces, secondary aerosolization possibilities, and the effects decontamination may have on the surfaces. Understanding the characteristics of both the pathogens and indoor environments will facilitate the remediation process, reducing the impacts on the economy and public health system. A systematic review of the scientific literature to obtain information on the fundamental characteristics of six biological agents, and an assessment of commercial indoor environments has been initiated. The agents, Bacillus anthracis, Yersinia pestis, Brucella spp., Burkholderia mallei, Francisella tularensis, and Variola major (smallpox virus), were chosen for their perceived likelihood of use and their diverse characteristics.

Cheryl Gleasner
University of Florida
B-6
Mentor: Chris Detter

Presentation Title: Genome Sequencing: Yesterday, Today and Tomorrow

Presentation Abstract: The Joint Genome Institute (JGI) is funded by the Department of Energy's Office of Biological and Environmental Research (OBER) to provide high throughput sequencing and computational analysis that enables genomic system based scientific approaches to DOE relevant challenges in biomediation, bioenergy and carbon sequestration. The JGI is comprised of five national laboratories, the Stanford Human Genome Center and the Production Genomics Facility. Los Alamos National Laboratory (LANL) is the JGI's main arm of genome finishing. JGI/LANL is composed of five teams that began mapping chromosome 5 and 16 more than eight years ago as part of the Human Genome Sequencing Project. Recently, JGI/LANL has focused on the wet lab and computational finishing needs of the JGI and has finished more than 100 microbial genomes in the past three years. Sanger sequencing, determines sequences by the use of dideoxynucleotides in a DNA polymerase catalyzed DNA synthesis reaction, has long been the preferred method of sequencing. Recently new sequencing technologies have emerged that incorporate pyrosequencing. Pyrosequencing produces sequences from the detection of released pyrophosphate during DNA synthesis. The newer methods produce shorter reads, more coverage and cost less to run than traditional Sanger methods. JGI/LANL uses both Sanger sequencing and pyrosequencing data to finish genomes. We are exploring the many uses and capabilities of our new GSFLX while working to develop new applications. In order to continue producing high quality sequencing data, the JGI must implement the new sequencing technologies into their sequencing pipelines.

Jessica Hammon
University of California, Santa Barbara
P-21
Mentor: Michelle Espy

Presentation Title: Deception Detection

Presentation Abstract: In December 2006, the National Defense Intelligence College (NDIC) released a report on the Science and Art of Interrogation. The Applied Modern Physics Group (P-21) has extensive research in measuring the magnetic fields generated by neural activity, "magnetoencephalography" (MEG), and is interested in correlating such brain activity with measures of so-called "lie detection." This project summarizes a few of the psychophysiological and neural mechanisms involved in deception, as reviewed by the NDIC and as relevant to the other MEG research in P-21. The psychophysiological mechanisms are divided into the autonomic (involuntary) and somatic (somewhat more controllable) responses often measured that include respiration, heart beat, and muscle contraction; however, other research involves the quantification of non-verbal cues, such as body movements, gestures, posture, eye gaze, and microfacial expressions. We briefly review the instruments used to measure such mechanisms, including the polygraph, eye tracking, and the Facial Action Coding System (FACS). The neural mechanisms measure more directly the brain activity itself, which requires a more thorough knowledge of the relationship between cognition and neural processes. We briefly review several imaging techniques, with particular emphasis on MEG and its electrical analog, electroencephalography (EEG), which are topics of extensive research in P-21. The NDIC report concludes that much research is still needed if these brain imaging techniques are to become operationally reliable and useful. Through research into the underlying neural mechanisms of deception and the possible correlation of these mechanisms with observable distinctions, we hope to provide a more scientifically grounded mechanism for the future of deception detection.

Philippe T. Levy
University of California, Berkeley
EES-2
Mentor: Nathan G. McDowell

Presentation Title: Respirate! An Analysis of CO_2 Efflux Versus Water Content and Temperature in New Mexican Soils

Presentation Abstract: The release of CO_2 from the soil surface is termed soil respiration. The two major sources contributing to soil CO_2 respiration are autotrophic, or plant root, and heterotrophic, or microbial decomposition. Worldwide, soils contain 1600 gigatons of carbon, twice that of the atmosphere. Soil respiration is the largest source of CO_2 to the atmosphere from terrestrial ecosystems, and is sensitive to climate factors such as temperature and soil water content (SWC). Thus, small climatic perturbations can cause large changes in the rate of respiration (CO_2 efflux) to the atmosphere, increasing greenhouse gas composition of the atmosphere and potentially feeding back on global warming. Most soil respiration studies report that CO_2 efflux is positively correlated with soil temperature; however, most of these studies have been done in humid climates where water is not a limiting resource. To investigate the climatic factors affecting soil respiration in semi-arid ecosystems, we measured we measured CO_2 efflux, SWC, and soil temperature at a piñon-juniper woodland located at Los Alamos National Lab (TA-51). The summer of 2007 was the third year of measurements made with a portable infra red gas analyzer and portable soil water content sensor. In contrast to most previous studies, temperature exerted a weak negative correlation and soil moisture exhibited a strong positive correlation with CO_2 efflux (R_2=0.008, p=0.75), and r_2=0.57, p<0.001) respectively). It appears that soil moisture, rather than temperature, is the critical driver of soil respiration in this semi-arid ecosystem, contrary to the more commonly documented, wetter ecosystems.

Erica Miller
University of Georgia
B-7
Mentor: David Fox

Presentation Title: Capture, extraction, amplification and detection of influenza A: Toward the integration of discrete biological steps on a single platform

Presentation Abstract: Of the three genera of influenza (A, B, and C), infection with the influenza A virus is the most severe and are currently causing a host of concerns in both the public and health sectors due to the potential emergence of a pandemic strain for which no vaccine is available. Specifically, the highly pathogenic strains associated with avian influenza virus (AIV), which may ultimately mutate to jump from birds to humans and, ultimately, from human-to-human, will demand rapid diagnosis. This is important not only for timely therapeutic intervention but also for the early identification of an influenza outbreak. Efforts in our laboratory to accomplish the goal of rapid detection of influenza A are currently in progress and consists of three major components: 1) Capture of influenza A virions and extraction of the vRNA genome through an immunological magnetic affinity-based enrichment step; 2) Isothermal reverse transcription (RT) and Helicase-dependent DNA amplification (HDA); and 3) Direct detection of the amplified product (amplicon) through a colorimetric visualization. The novelty of this technique resides in the integration of discrete biological steps onto a single platform and will require no instrumentation. Progress towards this end will be described.

Stephen Ortega
Northern New Mexico College
B-9
Mentor: Jim Freyer

Presentation Title: Chromosome Isolation

Presentation Abstract: The purpose of this project is to sort chromosomes from human fibroblasts showing a stable translocation induced by exposure to ionizing radiation. We want to sort the rearranged chromosomes in order to analyze the DNA sequence information at the radiation-induced breakpoint. The first sample we are working with contains a reciprocal exchange between chromosomes 2 and 4. In order to isolate the chromosomes, we added colcemid, an agent that disrupts spindle formation and arrests the cells in mitosis. After incubation the cells were harvested, swollen and lysed. We monitored lysis by adding a small amount of propidium iodide to the sample and observing the sample using a fluorescent microscope. Chromosomes are released from the mitotic cells after lysis of the outer membrane. The chromosomes are then separated from intact nuclei (from non-mitotic cells), stained with two different DNA fluorophores and sorted by flow cytometry. Following sorting the rearranged chromosomes will be sent to our collaborator, who will analyze them using a technique called array painting. In array painting DNA from the sorted derivative chromosmes is amplified and labeled, via the polymerase chain reaction, with a suitable fluorochrome (Cy3). The main purpose is to identify common sites of exchange between chromosomes in order to better understand the mechanisms behind radiation-induced chromosome rearrangements

Heath Powers
University of New Mexico
EES-2
Mentor: Nate McDowell

Presentation Title: Measuring Soil CO2 Fluxes and Stable Isotopes With a Chamber System and Tundable Diode Laser

Presentation Abstract: Stable isotopic analysis of carbon dioxide in the atmosphere has significant potential to elucidate the role of terrestrial ecosystems on global carbon and water dynamics. The concentration and stable isotope ratio of CO2 offers a powerful tool for understanding atmospheric-ecosystem interactions and the photosynthetic and respiratory processes that control these interactions. Isotopic analysis has until recently required samples to be collected in the ecosystem and returned to the laboratory for analysis via a mass spectrometer, a process that restricts the duration of the experiment and the number of samples collected for isotopic analysis. A tunable diode laser was used to make high frequency measurements in situ for measuring fluxes and stable isotopic composition of soil respired carbon dioxide. The chamber we tested is an open flow-through design where fluxes are calculated by measuring the differences in CO2 concentration between the air entering and the air exiting the chamber. A tunable diode laser (TGA100A, Campbell Scientific) was used to monitor the stable isotopic composition (δ 13C and δ18O) of the chamber's entering and exiting air streams and this data was used to model the isotopic component of the soil respired CO2. An experimental barrel using CO2 generated from gas with a known isotopic composition was used for chamber testing. The measured isotopic composition was within 0.9 per mil of the expected values for δ13C, and within 5.0 per mil for δ18O, and was independent of flux rate.

Crystal Ray
Massachusetts Institute of Technology
ENV-EAQ
Mentor: Leslie Hansen

Presentation Title: Riparian Area Surveys in Mortandad Canyon

Presentation Abstract: A riparian ecosystem contains a high diversity of plant species that contribute to its role, among many others, of preventing surface runoff, dissipating stream energy flow during high flow events, reducing undercutting and erosion, serving as a natural biofilter for improvement of water quality, and a food source for animals. It is dependent on perennial and ephemeral steams, rivers and the shores of other bodies of water. Riparian areas are negatively impacted by livestock grazing, introduction of nonnative plant species, human anthropogenic activities and occasionally, wildlife behavior. To monitor the potential for movement of pollutants from Los Alamos National Laboratory (LANL) areas such as parking lots and drainages, riparian area surveys were done in Mortandad Canyon to evaluate the current condition of riparian areas. The riparian areas were surveyed by choosing a representative plot of the riparian area, recording the plant species in one meter increments along the perimeter and determining the degree of undercutting and erosion. This data will help determine if riparian recovery efforts are needed so that future pollutant runoff from lab areas is prevented and downstream water quality improves.

Jesse Resnick
University of New Mexico and Westminister College
C-PCS
Mentor: Basil. Swanson

Presentation Title: Title: Waveguide based Optical Biosensor for the Detection of Disease Markers

Presentation Abstract: There is an imminent need for sensitive and specific methods for the early diagnosis of diseases like breast cancer (BC) and tuberculosis (TB). The survival rate improves significantly with early diagnosis. However, current detection technology is time consuming, intensive, insensitive and expensive. The Sensor team at LANL has developed a waveguide-based biosensor for the detection of biomarkers associated with disease. The carcinoembryonic antigen (CEA) is a glycoprotein whose presence in the protein-rich, low volume nipple aspirate fluid (NAF) from the breast is an indicator of BC. We have developed a sandwich immunoassay for the rapid (~15 min), sensitive (<500 fM) and specific (low non-specific binding) detection of CEA in serum and NAF . We propose to extend this approach to other BC markers, thereby establishing a rapid diagnostic for BC. The increase in multi-drug resistant (MDR) variants of TB has prompted the need for a rapid diagnostic. Preliminary studies in our laboratory have indicated that several Mtb-specific antigens are present in the urine of the infected host. We are currently validating these results and developing sandwich immunoassays for these antigens for use in the waveguide-format. This effort entails the selection of the appropriate antibodies, purification and labeling of the same and adaptation of the immunoassay. We have developed such a sandwich immunoassay for lipoarabinomanna (LAM) and antigen 85 (Ag 85 complex). We anticipate optimization of this assay and testing the same on urine samples from MDR TB patients.

Alayna Rodriguez
Harvard University
B-9
Mentor: Kim Chang

Presentation Title: Cloning of *M. tuberculosis* genes for the TB Structural Genomics Consortium

Presentation Abstract: *Mycobacterium tuberculosis* poses an increasing health threat to the global community, especially given the emergence of multi-drug resistant strains. Approximately 1.6 million people per year die from the disease; furthermore, 10 percent of the 2 billion people infected with TB bacilli will develop tuberculosis within their lifetime. In order to accelerate the discovery of antitubercular drugs, the TB Structural Genomics Consortium works to determine the three-dimensional structures and functions of *M. tuberculosis* proteins. *M. tuberculosis* gene cloning and protein production are central to this effort. The conventional cloning method relies on restriction enzyme digestion of both the target gene and vector, followed by ligase treatment. In a newly developed method, ligation-independent cloning (LIC), 3’ and 5’ overhangs on both the target gene and vector are generated by T4 DNA polymerase and then used in ligase processes to anneal the target gene into the vector. Finally, a point-mutation method can be used on the target gene to allow the engineering of more convenient restriction enzyme sites, thereby facilitating ligation. Using these techniques, we cloned several *M. tuberculosis* genes, including Rv2780 and Rv1843c, which were selected by the nucleotide ligand analysis method. The gene products of Rv2780 and Rv1843c are hypothesized to be involved in amino acid transport and nucleotide transport, respectively. Thus, the goal of this project is to confirm the roles of these genes in nucleotide metabolisms of *M. tuberculosis*. Other cloned genes include Rv2107/Rv2108, Rv3477/Rv1196, Rv1054/Rv1055, and Rv0285/Rv0286. Since these were predicted to form complexes by bioinformatics, we cloned two genes in one vector to see their interactions. In this poster, we discuss the cloning results of these *M. tuberculosis* genes.

Timothy Sanchez
Northern New Mexico College
B-8
Mentor: Srinivas Iyer

Presentation Title: Comparison of Proteomic Analysis Software

Presentation Abstract: (a) Purpose: The field of Proteomics is dependent on cutting edge technologies in mass spectrometry. In typical experiments, the amount of data generated is very large. This data set needs to be analyzed rapidly and manual analysis can be very tedious and time consuming, thus sophisticated software packages are being developed to analyze proteomic data. The intent of this project was to compare a few tools that can be utilized in proteomic analysis. (b) Procedures used: The raw data that was used in this project originated from peptide spectra acquired on a Q-star hybrid quadrupole-Time of Flight mass spectrometer. Program A, our existing software, has been in use for 5 years now and has allowed us to perform database searches using peptide mass fingerprinting and MS/MS ion searches. The raw spectra were analyzed using the established procedures and the results were tabulated. The new program (program B), which we wanted to evaluate allows us to gather further observations of the data and has features not available in Program A, such as de novo sequencing. We analyzed the same raw data set using Program B and compared the analysis results with that obtained with Program A. A Venn diagram was made that displayed the number of proteins identified by both programs and also those that were identified by one program alone. (c) Data: In data processing, using Program A and B, we found very distinct differences in our analysis. Program A was quick and proved to give valuable information on our data. Program B was very thorough in its analysis, providing some additional information not found by program A. This raised some critical issues in the analysis of our data suggesting that each software algorithm does result in some unique identifiers. (d) Conclusions: I concluded that ideally, we should utilize multiple programs to obtain the highest quality of analysis.

Amber Smith
University of Utah
T-19/CNLS
Mentor: Alan Perelson

Presentation Title: Within-Host Dynamics of Secondary Infections: Influenza and Streptococcus pneumoniae

Presentation Abstract: Secondary bacterial infections associated with influenza are a leading cause of death in the United States. These bacterial infections, mainly caused by Streptococcus pneumoniae, capitalize on the environment in the respiratory tract created by the Influenza virus. Experiments suggest a lethal synergism between these pathogens, but the precise mechanisms involved are unknown. However, some hypotheses attribute the interaction to specific viral properties, dysfunctional immune responses, and/or accelerated cell regeneration. In addition, an interesting and surprising observation is the change in viral levels following the bacterial challenge suggesting a truly dual effect. While the kinetics and interactions of these two pathogens are not well understood, we are developing ordinary differential equation models of the following three infections: (i) influenza, (ii) S. pneumoniae, and (iii) influenza followed by S. pneumoniae 7 days later. Using experimental mouse lung data, we are fitting the models, estimating parameters, and investigating synergistic mechanisms.

CHEMISTRY

Ernest Asani
New Mexico Highlands University
EES-6
Mentor: Hongwu Xu

Presentation Title: Design, synthesis and characterization of metal-organic frameworks based on the organic ligand 4-(1H-1,2,4-triazol-1-ylmethyl) benzoic acid

Presentation Abstract: Design, synthesis and characterization of metal-organic frameworks based on the organic ligand 4-(1H-1,2,4-triazol-1-ylmethyl) benzoic acid The subject of meta-organic frameworks (MOFs) has been an area of active study due to their potential applications in gas storage, molecular recognition and catalysis. The utilization of MOFs as storage materials for gas molecules, especially hydrogen, is the focus of this work. Hydrogen is regarded as the best alternative to the rapidly depleting and polluting fossil fuels. However, the design of materials with properties suitable for hydrogen storage remains very challenging. We have chosen the ligand 4-(1H-1,2,4-triazol-1-ylmethyl) benzoic acid (4-YMB) with a single monodentate carboxylic acid function as the organic linker to metal cations (e.g., Cd, Co and Zn) and have used a solvo-thermal method for the synthesis of 4-YMB based MOFs. The method involved a one-pot synthesis wherein the ligand, metal salt, and the respective solvents (water, dimethylformamide, triethanolamine, etc.) were mixed and sealed in a Teflon autoclave. The mixture was then gradually heated at a rate of 5 °C/min to about 120 °C for one day and cooled to room temperature at the same rate for another day. The resulted samples were characterized using powder and single-crystal X-ray diffraction and other techniques. These compounds may possess channels and cavities appropriate in size and shape for hosting gas molecules including hydrogen. The relative stability of these materials when their guest molecules are removed is also considered a desired property.

Sofiane Boukhalfa
University of Illinois, Urbana-Champagne
C-CSE
Mentor: Stephen Doorn

Presentation Title: Redox Chemistry of Carbon Nanotubes

Presentation Abstract: Single Walled Carbon Nanotubes (SWNT) have been under close scrutiny by the scientific community since their discovery in 1992 due to their surprising material properties. SWNT synthesis can be achieved in numerous ways. However, these methods result in a wide spectrum of chiralities of nanotubes. In order to more efficiently use these novel materials, individual chiralities must be isolated. To achieve this, a reduction-oxidation chemistry approach is used. Redox reagents of different electro-chemical potentials were added to solutions of SWNT in surfactant. Spectroscopy (absorbance and fluorescence) measurements were taken in order to monitor the effects of electron transfer between the SWNTs and the salts. Once chiral-specific doping can be achieved, isolation of these individual chiralities of SWNTs is planned through the use of ultracentrifugation. 20µL of each redox reagent was added to 3mL SWNT in surfactant solution while spectroscopy measurements were taken every 7 seconds in order to map out chiralities. Using a Fermi level map of the chiralities as a model, it was determined that the electro-chemical potential of the reagents directly affected the chiralities which were quenched during the experiments. Interaction between the salt and the surfactants is characterized by aggregation of the SWNTs; in the current redox reactions such aggregation, which broadens the spectroscopic signals, are not observed. Thus, a direct correlation was determined between the electro-chemical potential of the redox reagent and its effects on the nanotube solutions. This work establishes a future guideline for new work in the isolation of individual chiralities of nanotubes.

Christina Brady
University of California, Davis
C-CSE
Mentor: Steve Doorn

Presentation Title: Multiplexed Assemblies for SERS-Detection Application

Presentation Abstract: Raman techniques offer advantages over the well-established fluorescence in detection applications and microscopic analysis. Unlike fluorescence, Raman spectroscopy generates narrow peak widths allowing for a distinct fingerprint spectrum and easy identification of a material; however, low signal strength from Raman spectroscopy has limited its practical applications. Raman applications have increased with the use of Surface Enhanced Raman Scattering (SERS). To overcome weak signal strength, metal nanoparticles, such as gold or silver, are used as substrates for the attachment of the signal dye. Various attempts have been made to optimize the Raman signal by allowing the combination of different signal dyes for a single SERS-active nanoparticle. To achieve this, current research at Los Alamos National Laboratory involves synthesis of multiplexed nanoparticle assemblies to give a combination of signals. Silver (Ag) nanoparticles approximately 60nm in diameter were tagged with a particular Raman dye, aggregated, and silica coated. The tagged Ag particles were attached to silicon microspheres via biotin-avidin interactions in different dye ratios. Raman spectroscopy and Raman microscopy were used to measure and characterize the signal strength of the particles. Results showed that optimization of Raman signals occurred with the aggregation of Ag nanoparticles due to increased surface plasma resonance between the particles. Attachment chemistry of SERS-active nanoparticles to the silicon bead and dye combination spectra are currently being analyzed. Multiplexed nanoparticles can be used in further experiments requiring SERS-detection of different substrates simultaneously. Future synthesis of multiplexed particles with different combination of dyes will allow for a larger array of dye spectra than currently available

Laina Bretzke
University of Minnesota
PMT-2
Mentor: Anthony Lupinetti

Presentation Title: Liquid-Liquid Plutonium Recovery Using Ionic Liquids

Presentation Abstract: Currently the solvent extraction process for removing plutonium consists of the combination of two liquids; a feed containing hydrochloric acid, plutonium, and trace impurities; and an organic solution made up of n-dodecane and 1-decanol containing tri-n-butyl phosphate (TBP),. The organic solution has been used for some time and, while they do a good job of stripping the feed of plutonium, they have a number of disadvantages: they form a third, immiscible, phase under some processing conditions; they are combustible; and they are harmful to the environment due to their modest vapor pressures. In order to create a system that has more desirable properties, we selected two common room-temperature, ionic-liquids as replacement solvents for the current solvent extraction system being employed at TA-55 in the Aqueous Chloride Recovery Line. These ionic liquids are often referred to as "green" because they have negligible vapor pressures. We used 1-octyl-3-methylimidazolium and 1-decyl-3-methylimidazolium each reacted with lithium trifluoromethanesolfonimide. These reactions created two different ionic liquids which we can then contact with a feed containing plutonium in order to test the extraction process. We can then test different amounts of both the ionic liquid and the hydrochloric acid in the feed in order to find the most effective concentrations for the extraction process. Once these amounts are found this new process can then be used to more efficiently purify plutonium while saving time and resources along with protecting the environment. More research can continue this process in order to determine if other combinations of ionic liquids can be used to make the improved process more effective.

Lawrence Cai
Yale College
C-PCS
Mentor: Aaron Anderson

Presentation Title: Preparation and Use of Novel Organosilanes for Biosensor Applications

Presentation Abstract: Self-assembled monolayers (SAMs) consist of a single layer of molecules on the surface of a substrate. The available literature describes SAMs that have either of two desired features: binding functionality or non-specific binding resistance. For the purposes of an optical biosensor, a surface must have both of these characteristics. The use of phospholipid membrane bilayers in biosensors offers superior resistance to non-specific binding resistance but also has several disadvantages, including instability in air, instability to detergent rinse, and inflexible chemistry. To address the shortcomings of phospholipids, we have designed a SAM that combines both binding functionality and non-specific binding resistance. However, the creation of fully functionalized SAMs for use in biosensors can require up to two weeks to complete several steps. In order to streamline the process of creating SAMs, thus increasing the throughput of experiments, we developed a method to reduce the number of steps required to produce a SAM on the substrate surface. 3-Amino-propyl-triethoxysilane is a suitable platform for SAMs in optical biosensor but a longer alkyl chain may exhibit better binding functionality and non-specific binding resistance. To this end, we have synthesized 11-acetamido-undecyl-1-trichlorosilane, which is an advanced intermediate to the desired SAM product. This molecule can be deposited on any oxide surface and can be further functionalized for specific detection means, thus eliminating many of the steps that were previously performed on the substrate. Synthesis, deposition, characterization, and modification are described.

Jason Dugger
University of New Mexico
EES-12 ACRSP
Mentor: Jean-Francis Lucchini

Presentation Title: Study of some Chemical Properties of Hypohalites

Presentation Abstract: Researchers in the Actinide Chemistry Repository Science Program (ACRSP) in Carlsbad are conducting experiments to support the recertification of the Waste Isolation Pilot Plant (WIPP), the only working nuclear waste repository in the US. The chemistry of an underground nuclear waste repository can be affected by radiolysis. Hypohalite ions, like hypochlorite (OCl^-) and hypobromite (OBr^-) ions, can be radiolytically generated in brines, and can potentially oxidize key actinides stored in a repository, leading to enhanced subsurface mobility. The objective of this study was to determine some chemical properties of OCl^- and OBr^-. First, the molar extinction coefficients and wavelength absorbencies were found using UV-Vis spectrophotometry. Previous studies showed that hypobromite ions formed spontaneously in the presence of hypochlorite ions and sodium bromide. Further experiments were performed to support previous data as well as to confirm ideal molar ratios for formation of hypobromite ions. The pK_A values of the ions were determined using an automatic potentiometric titrator. The redox potentials of the hypohalite ions were also determined. The reactivity of the hypohalite ions with some key redox-active subsurface metals (iron, uranium) was also investigated. For example, the interaction between OBr^- and ferrous ion (Fe^{2+}) was studied using the ferrozine method. This project ultimately increases our understanding of the role that these key radiolytic products could play in the WIPP underground.

John Guido
West Virginia University
C-ADI
Mentor: Edel Minogue

Presentation Title: A Study of Decorporation Agents to be used in the Event of a Dirty Bomb

Presentation Abstract: Recently, following elevated terrorist threats, the concern of a dirty bomb attack on the United States has intensified. Such an attack would deliberately release radioactive elements into the environment which could then be incorporated into the bodies of victims by a number of routes. Once inside the body, if left untreated, many long-term, debilitating health effects such as acute radiation syndrome, cell death or mutation, and cancer can arise. Due to availability, relative ease of attainment, and inherent toxic properties, the radionuclides of major concern that could be used in such an attack are: Americium-241, Cesium-137, Strontium-90, and Cobalt-60. A decorporation agent is a chemical compound that lessens internal radiation exposure by reducing absorption and enhancing elimination of the radionuclide from the body. Several agents have been developed for the decorporation of each of the aforementioned radionuclides. However, limited efficacy, high cost of production and treatment, and an insufficient supply of these decorporation drugs in the National Stockpile are disadvantages that a mass casualty dirty bomb attack could easily exploit. With the evacuation of a target city being nearly impossible immediately following an attack, vast improvements in decorporation technologies are needed. New decorporation agents should be more effective than the current drugs of choice, while also maintaining ease in administration, be non-toxic, inexpensive to produce, and possess long shelf lives so they may be added to the National Stockpile and subsequently called upon if needed. This work evaluates the state-of-the-art for decorporation agents and suggests potential areas for improvement.

Jacob Izraelevitz
Franklin W. Olin College of Engineering
MPA-CINT
Mentor: Andrew Dattlemaum

Presentation Title: Determining the porosity of silica thin films using ellipsometry

Presentation Abstract: I constructed an apparatus for determining the porosity of thin film samples using data collected on a spectroscopic ellipsometer under controlled humidity conditions. We studied a variety of ordered nanoporous silica thin films that were prepared by an evaporation induced self-assembly process. Ellipsometric data, collected under controlled humidity conditions, was used to measure the thickness and index of refraction of the films. This data was then used to determine the pore size and distribution of each film. The nanoporous films were also functionalized with selfassembled monolayers and the porosity was calculated to determine to what extent the functional molecules entered the pores. This process may generally be used to calculate the pore functionalization of a variety of nanoporous materials.

Chandra Kluk
Fort Lewis College
IIAC
Mentor: Lia Brodnax

Presentation Title: Solution and Solid State Chemistry of Cerium (III/IV) in Alkaline Peroxide Carbonate Solution

Presentation Abstract: The carbonate ligand is known to form strong complexes with both actinides and lanthanides. Understanding the behavior of lanthanide (III) (Ln) in carbonate solutions is important for repository purposes and for understanding fission product behavior to aid in developing a new alkaline spent nuclear fuel process. Previously it was determined that the solubility limiting solution species for Nd was Nd(CO3)4 (H2O)5-, and the other trivalent lanthanide are expected to be iso-structural with the Nd species. The chemistry of Ce is more complex than the other light Ln due to its ability to exist in either its +III or +IV oxidation state. In carbonate solutions Ce (III) is oxidized to Ce (IV) forming Ce(CO3)56-, and in guanidinium carbonate Ce forms a dimeric Ce (IV) peroxo-carbonato structure with spontaneous in situ generation of peroxide. Three new polymorphs have been isolated and characterized by single-crystal X-ray diffraction studies. Two peroxo-carbonato dimer polymorphs were characterized as having the structure (C(NH2)3)8(Ce2(O2)(CO3)6) • nH2O (n = 6, 2). The higher hydrate (red/orange needles) forms first and after being left in solution for a few days converts into the lower hydrate (red plates). The pure carbonate species (C(NH2)3)6(Ce(CO3)5) • 4H2O was also isolated from these solutions. We will discuss the mechanism of the H2O2 formation and the complex chemistry of the Ce (III/IV) system in various carbonate solutions including: crystallographic data, photographs, spectroscopic characterization (UV-VIS, RAMAN, and FT-IR), and thermodynamic parameters for the relevant solution species (i.e. equilibrium constant and molar absorptivities).

Willie E. Montoya
PMT-4
University of New Mexico
Mentor: David A. Costa

Presentation Title: Removal of Trace Plutonium from Uranium Residues via Ion Exchange/Extraction Chromatography Systems

Presentation Abstract: The development of an ion exchange decontamination process for the removal of transuranics, specifically plutonium, from uranium oxide is of great importance to the nuclear complex. The decontamination efficiency of plutonium from uranium oxide in a nitric acid solution has been shown to vary based on the pH of the acid using different resins (Reillex HPQ Polymer and/or Bio Rad AG MP-1). This is possibly due to recontamination of the cleaned surface by residual Pu. During the decontamination process, uranium oxide is dissolved from the surface of the part, liberating undesirable plutonium oxide contamination from the surface. Increasing the pH of the solution into the basic region activates the vinyl pyridines in the resin to attract Pu ions onto the resin column and discriminate against uranium, which flows through the column. Decreasing the solution pH strips the Pu from the vinyl pyridines to be recovered. Our study was designed to determine the distribution coefficients [KDs] which were calculated for the different resins. The KD is a ratio of analyte activity in the resin phase to the solution phase. A high KD indicates high removal of the actinide species from solution. Additionally, for the nitric acid dependency studies, the separation factors (S.F.) were computed. Very high S.F.'s indicate that extraction of Pu is significantly better than U uptake and poor for very low S.F.'s. These were calculated for both uranium and plutonium in nitric acid solution to determine the efficiency of various resins at certain pH to remove the residual contamination from solution.

Dominique Price
New Mexico State University
C-PCS
Mentor: Aaron Anderson

Presentation Title: Aminopropylsilane-based SAMS: Stability Studies and Thiol Capture

Presentation Abstract: Biosensors use specific ligand interactions to detect target molecules, making them applicable to biomedical science as well as other biology fields. While phospholipid membrane bilayers work well at resisting non-specific binding, they do not satisfy some other expectations, such as stability over time, reusability, and flexibility with respect to the surface chemistry available. Replacing phospholipid membrane bilayers with SAMs has been relatively successful in the waveguide experiments. Our self-assembled monolayers are created by first attaching a silane to a glass slide by vapor deposition, followed by chemical modification with polyethylene glycol and the ligand biotin. However, we have not studied the stability of the SAMs in great detail. We report here stability studies of our SAMs in different environments; air, water, and buffer, and their degradation or stability over time using water contact angles. Another area of interest lies in the ligand we use. Biotin binds specifically to avidin, strepavidin, and neutravidin, but when we want to capture other molecules we have to find alternative ligands to use. Our attention has shifted to the capture of thiols for use in nucleic acid-based sensing. To capture thiols we attached iodoacetate to our SAMs instead of biotin. Fluorescence microscopy studies using a thiolated fluorescin derivative are shown. We plan to test the new SAM's ability to bind specifically to thiols with the use of the waveguide.

Scott Rabin
Massachusetts Institute of Technology
C-IIAC
Mentor: Jacqueline Veauthier

Presentation Title: Ligand Design for Long-Range Electronic and Magnetic Coupling Between Polynuclear Metal-Ligand Complexes

Presentation Abstract: Recent literature has elucidated the unique electronic and magnetic properties of bimetallic ytterbocene complexes with polypyridyl bridging ligands. Our focus has been on a series of bimetallic ytterbocene polypyridyl complexes that show varying electronic and magnetic properties depending on the bridging ligand geometry. For example, the 1,3-bis(terpyridyl)benzene ligand has proven effective in binding two ytterbocene centers, which has proven unique such that the ligand geometry inhibits coupling of the ligand radicals on the bridging ligand, yielding a triplet ground state to which the ytterbium spin can ferromagnetically or antiferromagnetically couple.1 An extension of this work involves the syntheses of polypyridyl ligands capable of binding three ytterbocene moieties, such as 1,3,5-tris(4'-terpyridyl)benzene, using transition-metal catalyzed aryl coupling reactions. The desired ligand would introduce a third ytterbium to the template with two potential properties of interest: the ytterbium nuclei can spin-couple and produce a single molecule with an extraordinarily high spin, or the nuclei can exhibit 'spin frustration.' Systems of this nature, to our knowledge, have remained unexplored, and the synthesis and characterization of trimetallic compounds with this type of ligand could lead to a more thorough understanding of the electronic and magnetic properties in ytterbocene polypyridyl complexes that could lead to applications in data storage and spintronics.

[1] Carlson, C. N.; Scott, B. L.; Martin, R. L.; Thompson, J. D.; Morris, D. E.; John, K. D. *Inorg. Chem.* **2007,** *46,* 5013-5022.

Pawan Rastogi
Columbia University
C-IIAC
Mentor: Michael Fassbender

Presentation Title: Recovery of Radioarsenic from Irradiated Se Targets and its Chelation with DMSA for Radiolabeling Purposes

Presentation Abstract: Although often referred to as toxic and poisonous, arsenic has proven to have many potential uses in nuclear medicine. Isotopes of arsenic, such as 74As and 72As, have been used in Positron Emission Tomography (PET). 72As is a positron emitting isotope with a 26 hour half life, and a mean positron energy (EB+mean) of 1.2 MeV. 74As (t½ = 17.7 d) emits both positrons and negatrons. These characteristics lead 72,74As to be promising candidates for being incorporated into radiopharmaceuticals. Such 74,72As-labeled radiopharmaceuticals can be used in quantitative imaging of different biochemical and physiological processes. Two possible delivery routes for radioarsenic are considered: The direct production of longer lived radioisotope (like 74As), and the production of a radionuclide generator parent like 72Se, which, in turn, will decay into 72As. A potential portable radioarsenic generator will be of value due to transportability and efficacy in delivering the radioisotopes to hospital settings. Direct production of radioarsenic and the generator parent 72Se will be accomplished by irradiating a steel-encased 40 gram selenium target with a 100 MeV proton beam at the Los Alamos Isotope Production Facility (IPF). The main objective is the recovery of radioarsenic from the irradiated target material. Impurities like isotopes of germanium, gallium, and bromine are expected to be present. It has been proposed that separation of the arsenic can be accomplished by dissolution of target material, followed by a reduction and distillation of arsenic in its trivalent chlorinated form (AsCl3). It is projected that the distillate be further purified using a strongly basic anion exchange resin. It is also expected that 72Se will be formed in the target. By finding fast, efficient, and cost-effective methods of separating arsenic from selenium followed by a subsequent chelation of arsenic, the medical isotopes can be provided to pharmaceutical companies; either directly by shipment of 74As or as an 72As generator on-site. Following isolation of arsenic and its chelation, a biologically deliverable form of the isotope is hoped to be discovered. Due to time constraints, targets were not able to be irradiated. As a result, chelation of arsenic with dimercaptosuccinic acid (DMSA) is currently being developed using 75Se and 74As tracer activities. The purpose of this paper is to propose both arsenic separation methods and the chelation of arsenic with DMSA.

Courtney Walsh
FVCC
DE-9 & X-3
Mentor: Dana Dattelbaum

Presentation Title: Shock Chemistry Analysis of Tert-butylacetylene and Trimenthysilylacetylene

Presentation Abstract: Shock chemistry analyzes chemical compounds and reactions under extreme pressures generated by a shock front. It is necessary to understand these properties when dealing with explosives so that the desired reaction is achieved. Simulations and experiments have been run to see the static high pressure spectra of acetylenes, with a focus on getting the data from experiments to match what simulations predict. Static high pressure spectra data has been collected for tert-butylacetylene and trimenthysilylacetylene. Previous simulations of these experiments have shown some discrepancies that we wish to investigate and possibly explain.

Kevin Williamson
University of Wisconsin
C-IIAC
Mentor: Lia Brodnax

Presentation Title: Chemistry of U(VI) and Lanthanide (III) Complexes in Alkaline Carbonate-H_2O_2 Solutions

Presentation Abstract: Recent discoveries in differences of solubility and solution speciation of the Lanthanides (Ln) and Uranium (VI) in carbonate solutions have the potential to be used to develop a new alkaline-based separation process for spent nuclear fuel reprocessing. In particular, carbonate systems in the presence of hydrogen peroxide have displayed promise in the possibility of separating the Lanthanides from Uranium. We have previously shown that the peroxide ligand competes with carbonate in Uranium systems, and can form multiple mixed U-peroxo-carbonate complexes with higher solubility than pure Uranium carbonate species: $UO_2(CO_3)_3^{4-}$. The Ln behavior with mixed ligands was not known; however, it has been found that Lanthanides also form peroxo-carbonate complexes, but with lower solubility than their corresponding carbonates. Also, it has been demonstrated that peroxide preferentially binds Uranium in U/Ln mixed metal systems, while it competes for complexation of both U/Pu in their mixed metal systems. This behavior reinforces the possibility of an actinide separation from the lanthanides using the alkaline-based separation process. We will discuss the complex chemistry of Ln(III) in carbonate as well as U(VI) and Ln(III) in carbonate with H_2O_2, including structural characterization, thermodynamic parameters, and solution speciation.

COMPUTING

Laura Ambrosiano
Kansas City Art Institute
IST/OCIO
Mentor: Katherine Norskog

Presentation Title: Improving Web Visibility for National Security Story

Presentation Abstract: Since a great deal of Web traffic comes from search engine referrals, one of the best ways to improve the number of page visits is to make the Web site more visible on the main search engines. This means that the laboratory's page should appear on one of the first three pages of a search. My project is to assess the visibility of our national security story on Google, MSN, and Yahoo. By collecting quarterly statistics and conducting a search engine audit, I will understand the Web site's current status and derive plans for improvement. Since we want to ensure this site is a useful resource for policy makers, sponsors, and academics, I'll also be quantifying the origins of the visitors by domain. With the results of this analysis, I'll then be making informed improvements to the site, freshening the content, and adding links to related outside reading. We'll want to see improvement in the placement of the national security site within the next quarter. I'll then be documenting the process used to evaluate and improve our national security site presence on the Web so that similar plans can be used to improve other areas of www.lanl.gov.

John Auxier
Northern New Mexico College
C-AAC
Mentor: Donivan Porterfield

Presentation Title: C-AAC MTE Equipment and Chemical Standards Database

Presentation Abstract: The necessity for accessible, current standards in measurement equipment and chemical standards becomes a valuable asset to the division that does experimental work with items that require calibration. The purpose of this poster is to identify the difficulties that were overcome through the development of the M&TE and Chemical standards database. The major difficulty was the amount of relevant data that had to be extracted from the large amount of data available. A second difficulty encountered was in relating the equipment and chemical information from dissimilar sources into a common database with a unique format. This poster will also cover the major achievements completed in the development of this database; among these achievements is the capability to sort through all of the records of standards calibration history with a system that can generate reports of MTE or chemical standards that are approaching their calibration renewal cycle or the disposal date. This capability ensures that C-AAC standards equipment is current and accurate in its measurement capability. Other capabilities of the database is its abilty to give the users an interface to accurately track and record the different chemical and equipment standards and deliver the ability to input new chemical or equipment data and calibration dates and standards in a user-friendly environment. Finally, this poster will summarize the challenges that were met and overcome in the development of this database and demonstrate how these challenges are similar to the overall challenges that face the scientific community in the development or perfection of new technology.

Martin Baker
University of New Mexico
HPC-1
Mentor: Cecilia Sanchez

Presentation Title: Software for Humans

Presentation Abstract: The tagline of Lifehacker, the 6th most popular blog as measured by Technorati, says "Computers make us more productive. Yeah, right". Although presented in tongue-in-cheek fashion, the power of computers and the information they provide us can reduce productivity if the tools we use to harness them become unwieldy. User-centered software development focuses on making those tools easier to use and better suited to accomplish our goals. Designing software for humans involves focusing on doing one thing for the user and doing it very well. The user will have a specific set of expectations or requirements as part of that thing and these should be implemented with the user in mind. User testing is sometimes criticized as being a time-waster, but when good software engineering principles are used to develop software, the lifetime cost of the software decreases significantly and user acceptance increases. Designing software for the humans who use it produces software that is functional at heart instead of flashy. By involving customers early in the development process, software designers can build on a functional base by adding only those flashy features that will actually improve the user experience. The end result is soundly-built software that makes the customer happy and is easy to maintain.

Michael R Barela
University of New Mexico
MQ-3
Mentor: Tom Moxley

Presentation Title: Installation and Maintenance of Thermo-Hygrometer System for Standards & Calibration Laboratory

Presentation Abstract: In order to make measurements that adhere to national standards the LANL Standards & Calibration Laboratory (S&CL) must meet certain temperature and humidity requirements. To do so the S&CL must register with an accredited organization such as the National Voluntary Laboratory Accreditation Program (NVLAP). The S&CL has submitted a proposal to NVLAP for accreditation, which requires our organization to follow the ISO-17025 guidelines. First a set of requirements had to be established by the LANL S&CL. Then a suitable commercial system was purchased to monitor the temperature and humidity parameters. The system consists of a Fluke-Hart Scientific Dewk thermo-hygrometer unit with high accuracy sensors, server and clients. The Dewk units use a dedicated server to manage the system. The server was installed first and static network IP addresses were assigned for each unit. Then the Computing, Communications and Networking (**CCN**) Division was contacted to allow the Fluke LogWare Server and client applications access to our server. Then the firewall and file sharing capability was enabled so the Dewk units could communicate with the server and client software. The client software was installed on dedicated computers in each laboratory. Then the thermo-hygrometer units were plugged into the network and tested with the client software. Lastly, the client software was configured to communicate with our MetCal programming language software. The server of the initial system used had communication problems with the Dewk units. Then the client software had problems communication with the MetCal software. These problems were solved with technical support and patches supplied by software engineers from Fluke. The completion of the monitoring system will enable the Standards & Calibration Laboratory in achieving NVLAP accreditation.

Scott Blauert
New Mexico State University
IST-APPS3
Mentor: Brian McCool

Presentation Title: The Facility Browser

Presentation Abstract: In the high explosive exclusion area of Technical Area 9, there is sometimes a need to find specific about a certain building, room or piece of equipment. The current method to disseminate this information to workers is through a distributed book. The process of updating the book, printing it, and distributing it to workers is slow and time-consuming. A lot of relevant information and media must also be omitted due to limited space requirements. A web application which makes it easy to view and update information relevant to facilities was created. The application, which was written in .NET, gives web-browsing users a structured, tree-like navigational hierarchy of pages each assigned to buildings, rooms and pieces of equipment in TA-9. Every page and every item on each page, whether it be contact information, a note, or a picture corresponds to an entry in a SQL Server database. Updating the information is also done through a web-browser, using a separate application which makes changes to the same database. Ultimately, workers themselves will have the capability to make changes to data sheets for which they could be considered experts. The application currently only has information for TA-9, but there is no restriction on adding information about other Technical Areas.

Colby Boyer
University of California, Berkeley
HPC-5/CTN-5
Joseph Lopez
University of New Mexico
HPC-5/CTN-5
Kimberley McCormick
New Mexico Highlands University
HPC-5/CTN-5
Mentors: Robert Martinez, HB Chen

Presentation Title: Comparison of 10GigE and InfiniBand Interconnects

Presentation Abstract: The goal of a high performance supercomputing cluster is to achieve the highest possible performance using generic parts to the lowest cost. InfiniBand is currently used to maintain low latency and high bandwidth though the recent 10GigE standard offers considerable improvement over its predecessor in both bandwidth and latency performance and might be a viable option. Our driving question is whether or not 10GigE will be price and performance competitive with InfiniBand. Our objective is do a comparison between two cluster interconnect cut through switches: InfiniBand and Fujitsu 10GigE. This will be done by benchmarking the latency performance, throughput performance, cost, and scalability using MPICH2 over InfiniBand over IP and MVAPICH2 over native InfiniBand. We hope our results will show whether 10GigE is a viable interconnect for high speed computing applications.

Ekaterina Davydenko
University of New Mexico,
Kevin Krutsch
Michigan technological University
Dustin Balise
New Mexico State University
HPC-5
Mentor: Hsing-Bung Chen

Presentation Title: Xen Virtualization in an Enterprise Cluster Environment

Presentation Abstract: The purpose of this project is to scale a Linux cluster from a testing environment to a full scale enterprise. We are currently working with a cluster of ten nodes, one as the master control node where all of our main services dwell, such as DHCP, DNS, LDAP, NFS, and Nagios (a monitoring application). Each of these machines currently runs two AMD Opteron 250 CPU's accompanied by two gigabytes of RAM. The main purpose of this cluster is to serve as an entity to run MPI programs including benchmarking software, then to compare results with our fellow teams to see who achieved the best results. Our particular assignment is to use Xen virtualization software to simulate a larger cluster; we are aiming to simulate around a one hundred node super cluster. We are planning on upgrading the hardware configuration of the machines from originally installed two gigabytes of RAM, to four gigabytes of RAM per node to ensure that we have enough system resources available to support the amount of virtual nodes that we are planning on implementing. This project purpose is to see how virtual nodes effect the scaling capabilities of these benchmark software applications across the cluster. Do modern day super clusters really need to be as massive as they are, or can we use the aid of virtualization to minimize the amount purchased nodes? This method of virtualization can be very useful prior to purchase when planning a cluster implementation; with this method you can test your targeted applications to see just how many nodes you actually need. That was from an economic point of view, and another aspect of this research is to see exactly where these applications reach their performance threshold. Exactly when does a certain function reach its peak performance? After how many added nodes performance of application doesn't change? Tests also will include the scalability of Xen itself, meaning how Xen scales with different types of hardware, and when it starts to lack performance due to lack of hardware resources. All this is applicable when determining software we are hoping to provide an efficient aspect of testing prior to cluster implementation.

Paul S. Ferrell
New Mexico Insitute of Mining and Technology
CTN-5
Mentor: Mike Fisk

Presentation Title: Secure Communication System for FRNSE

Presentation Abstract: The Framework for Responding to Network Security Events (FRNSE) is a next-generation network intrusion detection system that is currently being developed by the CTN-5 Dart team. FRNSE gathers alerts from a wide variety of intrusion sensors spread across a network, attempts to correlate those alerts, and then takes action as appropriate. The sensors previously sent their alerts to the FRNSE server by using syslog to write the alerts to a remote log file. This insecure, unstable, and highly limiting method of communication needed to be replaced. We developed a secure communications module for FRNSE that provided SSL certificate authentication for both the sensors and FRNSE server, robustness in the case of communication failure, a flexible protocol, and an easy to use interface. Many sensors have already been successfully switched to this new module, and the old syslog communication method is expected to be entirely decommissioned by the end of the summer.

Jeannette Figg
UC-Santa Barbara, IMMS,
Amanda Larson
Los Alamos HS, CCS-1
Heidi Lewis
Colorado School of Mines, CCS-1
Mentors: Debbie Wilke, Cindy Sievers & Cindy Sievers

Presentation Title: Worldwide Collaborative Environments

Presentation Abstract: Communicating seamlessly with people around the world has become necessary, making computers an essential communication device. The increasing efficiency of the Access Grid software and ParaView systems make them ideal for this worldwide connection. Access Grid contains a variety of multimedia displays used in presenting data. Using Grid middleware to support group-to-group interactions allows worldwide conferences and enhances educational opportunities. Jeannette Figg works with the distance education aspect of the Access Grid. It offers students many options they would not traditionally have. Meeting with famous professors and enrolling in classes at distant universities are examples of the educational capabilities on Access Grid. Continuing improvement of the technology used with Access Grid is essential to maintaining and expanding its capabilities. ParaView uses a programming language similar to C++ and acts as a Visualization Toolkit (VTK) to simulate two or threedimensional objects and data sets. Combining ParaView and Access Grid will simplify the process of sharing and viewing data. By collecting statistics for Access Grid events, Amanda Larson and Heidi Lewis have helped build an integrated ParaView/Access Grid node connected to the Powerwall. This device visualizes and displays high-resolution data. It enables scientists to interactively view a data set from any angle and any method of visualization. This provides a large display area to host collaborations of small groups of researchers using the same data. We have been able to grasp a firm understanding of these systems by participating in several Access Grid meetings, and running demonstrations on ParaView and Powerwall.

Samuel Gutierrez
University of New Mexico
HPC-4
Mentor: David Montoya

Presentation Title: Increasing the Long-Term Viability of Open Source Performance Analysis Software

Presentation Abstract: A common thread that all successful open source projects seem to share is a synergism between a passionate developer base and an equally active user base. In order to help establish long-term viability, however, an open source project must first provide certain mechanisms and materials needed to foster a social network of adopters who will become active project contributors. The need for establishing this network is especially vital for those organizations who have a vested interest in the open source software project. OpenSpeedShop, an open source performance analysis framework based on dynamic instrumentation technology, is co-funded by the Department of Energy and is in the process of being integrated into the performance analysis tool suite utilized at Los Alamos National Laboratory, Sandia National Laboratory, and Lawrence Livermore National Laboratory. OpenSpeedShop allows for different collectors to be integrated into code regression suites to help categorize resource use and bottlenecks. The research and development focus at Los Alamos National Laboratory has been geared towards maintaining and extending OpenSpeedShop for use in secure high-performance computing environments. In particular, development has revolved around extending the base framework, refining the installation process, contributing to end-user/development documentation, and creating automation utilities and materials which introduce OpenSpeedShop's capabilities to potential users.

Yousef Iskander
Virginia Tech
CCS-1
Mentor: Justin Tripp

Presentation Title: Compiling for Reconfigurable Processors

Presentation Abstract: Recent releases of commercially available reconfigurable coprocessors, such as those offered by DRC Computer and XtremeData, utilize the newly published HyperTransport Protocol to create peer-to-peer connections between an AMD Opteron processor and an FPGA. By directly attaching to the HyperTransport bus, lower latency communication channels and global, shared memory between the processor and FPGA are now possible. These products allow FPGAs to be used in conjunction with low-cost, commodity hardware creating a flexible approach to building a reconfigurable computer. This research continues the work of Trident, a compiler for reconfigurable architectures. We aim to allow the integration of reconfigurable architectures, variable-latency memories (DRAM) and a host processor. The peer-to-peer connection offered by these reconfigurable coprocessors should reduce the communication cost between the sequential processor and reconfigurable coprocessor, thus allowing us to re-evaluate the trade-offs previously made when porting applications.

Joseph Izraelevitz
Washington University, St. Louis
HPC-5
Mentor: Josip Loncaric

Presentation Title: Analyzing Software Dependencies on Supercomputers

Presentation Abstract: Supercomputers are a key component in achieving the Los Alamos National Laboratory's mission. They are tools that apply to almost all fields of research, and allow scientists to explore previously unknown territory though enormous calculations. Because of the sheer demand on the computer, reliability is critical, as downtime is costly in both dollars and research; yet because of the scale of these machines, it is often difficult to track down problems that may not emerge on smaller systems. This complexity drives the development of software to make predicting, finding, and solving problems easier. All software programs rely on other programs, a relationship called a dependency. On the average desktop machine the web of these dependencies can contain several thousand relationships, and a supercomputer has more. However, if a single program breaks, any other program connected to it may also fail. Rev is a piece of software designed to make analyzing this web of dependencies easier. Taking advantage of the Red Hat RPM system, it allows the user to map dependencies in a visual way, view specific pieces of the graph, and track the dependency network through time. By better understanding how software packages interact, problems in supercomputer software can be solved faster and more completely.

Brian Kiedrowski
University of Wisconsin, Madison
X-3
Mentor: Roger Martz

Presentation Title: Implementation of CAD-Based Transport in MCNP6 Using GMC Capabilities

Presentation Abstract: Monte Carlo radiation transport simulation packages such as MCNP have become more prevalent for performing nuclear analysis as computing power advances. Increased demands on geometric detail and the desire to use the same geometry model in multiple physics codes have led to the use of CAD (Computer Aided Design) models as a basis for problem geometries. The DAGMC (Direct Accelerated Geometry-Monte Carlo) library developed at the University of Wisconsin-Madison in conjunction with work on CUBIT at Sandia National Laboratories was implemented as an option in MCNP6. DAGMC takes a CAD geometry in the ACIS file format produced by CUBIT, reduces the surfaces to facets, and puts the facets in a hierarchical data structure for efficient ray intersection queries. MCNP6 uses the facet data structure in the transport process whenever geometric queries are required in "DAGMC mode". Test problems were developed based on some experimentally validated MCNP Neutron and! Photon Benchmark Problems. Results of DAGMC-MCNP6 versus standard MCNP6 were compared and shown to be consistence. Unstructured, tetrahedral mesh features available in DAGMC were implemented to allow particle history tracking and tallying on the mesh to assist in coupling with finite element analysis packages.

Carl Knauss
Michigan Technological University
CTN-DO
Mentor: Fatima Woody

Presentation Title: Lujan Center PIX Firewall Project

Presentation Abstract: The Lujan Center PIX Firewall Project is an effort to help illustrate the configuration and function of the network security policies at the Lujan Center. In order to satisfy requirements of a DOE/LANS directive and the Yellow Hardening Project, the PIX Firewall's mission controls access to the Yellow Network by foreign nationals. To help ensure productivity and success to mission critical functions at the Lujan Center, the PIX firewall grants limited access to all hosts and subnets. Due to the overall complexity of the security policy put in place it is difficult to understand the administrative restrictions placed on users and hosts. The goal of the project is to help users and administrators understand the security policy configuration in order to better ensure mission success.

Nicholas Kutac
New Mexico State University
MC-PC
Mentor: Nancy Fresquez

Presentation Title: Oracle MRP Implementation for Pit Manufacturing

Presentation Abstract: The Manufacturing Processes Production Control (MC-PC) team has been implementing Oracle Discrete Manufacturing since January 2004. Oracle Discrete Manufacturing (DM) is a powerful suit of software solutions created to support manufacturing processes, but lacks a simple, intuitive interface designed specifically for shop floor use. Historically, other software companies have focused on solutions designed specifically for deployment on the shop floor. These solutions have been called Manufacturing Execution System (MES). Many MES systems can interact seamlessly with the Oracle Applications. These commercial off the shelf systems are often referred to as “bolt-ons” because of their inherent integration in design. These products may be able to assist on the shop floor to create user friendly interfaces for the Pit Manufacturing process. An in-depth analysis of the Oracle Partner companies and recent acquisitions should reveal the current state of the business from which a path forward can be decided on. The results expected from this study include: an analysis of the Oracle DM Bolt-on business and a decision on the best path forward for Oracle DM in Pit Manufacturing. If a user friendly interface were located and installed into Pit Manufacturing, the efficiency of the process would be expected to increase because users would not have to learn a complex computer system. Instead, they would use a simple interface which would enter data directly into the database while providing simple clean access for Pit Manufacturers.

Veronica Lopez
University of New Mexico
CTN-5
Mentor: Evelyn Roybal

Presentation Title: NERF - *NE*twork *R*egression test *F*ramework

Presentation Abstract: The main goal of a computer scientist is to discover ways to make life easier with the aid of computers. Therefore, I was given the task to alleviate the testing phase of software development. The NEtwork Regression test Framework (NERF), which is written in Scheme, was created to help resolve this issue. In general, regression testing begins after a programmer has tried to fix a known bug in the code or has added code to the program which resulted in unintentionally introducing errors. It is a method to verify that the recently modified code still fulfills particular requirements. It also ensures that unmodified code has not been affected by the changes. My concept with NERF was to create the framework that would allow a programmer to quickly complete regression testing on a program without having to write the lengthy client code. Instead, the programmer will write a simple script tester file which will be sifted through by my interpreter to determine if the code is fulfilling its purpose. My ambition is that NERF will benefit Los Alamos National Laboratory (LANL) by providing programmers with an easier way to test so they may concentrate on the actual coding phase rather than the testing phase of the software development life cycle.

Aaron Lovato
New Mexico Insitute of Mining and Technology
CTN-5
Mentor: Sandra Turner

Presentation Title: The Framework for Responding to Network Security Events: Protecting Data on the LANL Network

Presentation Abstract: The purpose of the Framework for Responding to Network Security Events (also known as FRNSE [pronounced fren-zee]) architecture is to monitor network event logs from the Laboratory's network sensors and respond to logs that indicate a security risk. With all of the sensors deployed around LANL, network security analysts face a difficult challenge in monitoring the high volume of logs from these sensors, determining whether an event is important, and then taking action to remedy any security risks indicated by the event. FRNSE automates this process by using agents to monitor logs from sensors and generate alerts from the data in these logs, which are then sent to the FRNSE server. We currently have agents to support 8 network sensors including Snort, Tipping Point, Sygate, and R3000. Once an agent sends an alert to the FRNSE server, the server puts the alert into a database and then may correlate the alert with other alerts or other data before sending it to the Rule-Based Response system. The Rule-Based Response system uses policy to determine the appropriate response to an alert. Current response mechanisms include posting a ticket for network security analysts, activating an internal block, activating a temporary internet block, and registering a vulnerability. By automatically taking action on some of the more severe alerts, we are able to both shorten the time necessary to respond to alerts as well as reduce the workload on our network security analysts. Future tasks include developing agents for more sensors, improving our alert correlation ability, and tuning sensors to be able to detect more security risks.

Kimberley Lucero
College of Santa Fe
CTN-5
Mentor: Rick Romero

Presentation Title: Telecommunications Project

Presentation Abstract: The Network Support Team designs, develops, installs, and maintains the Laboratory's computer networking infrastructure and maintains a Network Operations Center. The network responsibility covers both the primary communications system networks that interconnect the Laboratory's local area networks and the networks that support supercomputer and centralized resources. The primary job assignment for this position is to develop a web based database which will include working on a Telecommunications project to track the various switches in locations within the laboratory, also tracking all the spares equipment for ordering.

Adam Manzanares
University of Colorado
CTN-4
Mentor: Steve Howard

Presentation Title: Wireless Penetration Testing and AirDefense Response

Presentation Abstract; Wireless networking for Los Alamos National Laboratory is currently not allowed on any of the property unless special approval has been implemented. There is an approved wireless network for Occupational Medicine using WPA and a proposed captive portal system that would be used for a wireless network connected to the visitor network. Currently there is an installed base of 312 sensors which monitor the airwaves for any suspicious wireless activity. These sensors form a part of the LANL AirDefense system. This study aims to perform wireless attacks to determine how secure proposed solutions to wireless security are. The AirDefense system will also be watched to determine the response to these attacks. Planned attacks are: man-in-themiddle, SSL spoofing, MAC/IP spoofing, WPA cracking and Denial of Service. These attacks will be performed on a captive portal and also on a WPA pre-shared key network. The goal is to determine the amount of time and effort required to launch these attacks and to determine their signatures within the AirDefense system.

Daniel Mason
Tom Bowidowicz
Karen Ho
Arick Wang
Zach Kenyon
George Swinhoe
Lisa Alexander
Landon Sutherland
Los Alamos High School
X-3
Mentor: Marv Alme

Presentation Title: Summer Workshop on Mining Legacy Fortran Code

Presentation Abstract: This poster summarizes student activities at the Summer Workshop on Mining Legacy Fortran Code. This workshop, organized by the ASC Integrated Codes Program and X Division, was targeted towards current junior and senior students at Los Alamos High School. During this 5 week workshop, students received intensive training in Fortran programming, software configuration management tools (Subversion and CVS) and unit testing concepts. Following an initial phase of instruction, workshop participants organized into teams and worked to incorporate the legacy code (an ICF code written in the 1970's and early 1980's) into a code repository, restructured selected subroutines and wrote test drivers for these selected subroutines. Each team will present an example of reworked code, a test plan, and testing results. Workshop participants found the code challenging to read and understand because of short, non-descriptive variable names, frequent reuse of temporary arrays, awkward control loops, inadequate comments and no indentation. This workshop, a pilot program by X Division and the LANL High School Coop Student Program, was a partnership between LANL, Los Alamos High School, and the local business community. Much of the workshop, which was held in LAHS's Computer Loft, was taught by Todd Yilk, LAHS Computer Science Department.

Rey-Lynn Medina
David DeHerrera
University of New Mexico-Los Alamos
CTN-3
Mentor: Lanorra Sena

Presentation Title: PDMLink

Presentation Abstract: Product Data Management (PDM) Link is a new product definition, configuration management, and collaboration tool being implemented across LANL's Design and Production Agency. PDMLink is the first data management system that retains Computer Aided Design data parametric relationships while providing configuration management and control to other document types. These techniques are being conducted on a daily basis by CTN-3 students REY-LYNN MEDINA and DAVID DEHERRERA along with other members of CTN-3 and W-Division in order to implement moving files, email functionality, and locating files in PDM Link. Using these methods we are able to efficiently search, move, and email a folder or project to another. In conclusion, we are using PDM Link in order to successfully manage LANL's data. With this in mind we would like to make all LANL employees aware of PDM Link procedures so we can implement it to its fullest and ensure LANL's security.

Dylan Merrigan
New Mexico Insitute of Mining and Technology
Caleb Morse
University of New Mexico, University of New Mexico
Sherry Salas
New Mexico Highlands University
CTN-4
Mentor: Susan Coulter

Presentation Title: Advance Health Monitoring of Computer Clusters

Presentation Abstract: As the number of nodes and processors in a cluster grows, its interoperability and networking become more complex. This complexity drastically increases the amount of system errors and decreases performance. To ensure the accuracy and speed of a cluster, it is important the system be monitored and managed in an efficient and effective manor. Monitoring tools must quickly and correctly recognize performance degradation in clusters without requiring excessive system resources. They must also communicate with system administrators promptly to avoid smaller issues turning into systemwide problems. Our solution incorporated Nagios, a monitoring software, and Cacti, a graphing program, along with homegrown monitoring processes to track a small cluster's performance. Failures and delays will be injected into the system, such as unnecessary daemons and network errors, to ensure monitoring tools are providing swift and correct 07data.

Susan Meyers
University of New Mexico
CTN-5
Mentor: Victoria Varela

Presentation Title: The Anatomy of a 0 iframe Exploit

Presentation Abstract: Web-based exploits are continuously increasing ¬¬¬ in complexity and in proficiency at avoiding detection by security tools and antivirus software. These attacks exploit vulnerabilities in web browsers, operating systems and various software applications. The vector of infection can be a specially constructed email or a visit to a compromised website. Once a vulnerable system is exploited, a Trojan horse can be installed to steal personal information and/or to use the compromised system to attack other computers. In this study, attack vectors using 0 Iframes have been analyzed to determine the method of operation being used, the current trends and patterns for vulnerabilities being exploited, the effects of such attacks on the LANL network, and the determination of a proactive approach to minimize the impact of these attacks.

Larry Ortiz
University of New Mexico
CTN-2
Mentor: Aggie Naranjo

Presentation Title: Bart's Preinstalled Environment (BartPE) Utility CTN-2 version 5.1

Presentation Abstract: Los Alamos National Laboratory system administrators are always looking for ways to make their jobs easier and more efficient. A new utility was developed from Bart's Preinstalled Environment (PE) Builder and resulted in CTN's version of the utility, Bart Preinstalled Environment (BartPE) 5.1. The objective of my project is to explain the helpful utilization of CTN's version of BartPE. This version was created by Chris A. Casillas, CTN-2. A brief description about the origin of BartPE and what it is will be introduced. A short description of the software used to create a BartPE disk, Bart's PE Builder, and a run through of the steps required to initialize the BartPE disk will be highlighted. BartPE has additional plug-ins that can be added when customizing a BartPE build however, I will elaborate on the applications and utilities that are installed in CTN's version of BartPE; such as Network configuration, Ad-aware, Symantec Ghost, Password Renew, Secure Screen, Stinger, etc. Additionally, I will summarize a brief description of each application and/or utility included in CTN's version of BartPE. Topics covered will include the valuable uses of BartPE, such as recovering data, imaging a PC, virus cleaning, etc. The advantages of using BartPE over DOS-Based boot disks will be discussed.

Parimal Parag
Texas A&M
CCS-3
Mentor: Sami Ayyorgun

Presentation Title: Achieving Desired Buffer Occupancy for a Single-Server Queue

Presentation Abstract: We propose a probabilistic traffic-regulator (or servicecontroller) for satisfying stochastic QoS guarantees. We also present an algorithmic approach for generating a synthetic traffic such that when buffered in a queue with a time-varying service rate, the queue is stochastically bounded above by a pre-specified function. This traffic regulator is the probabilistic generalization of Leaky-Bucket Regulator. The proposed algorithm is simple to implement and has applications in end-to-end probabilistic QoS guarantees, study of priority queues, and realistic simulation studies.

Greg Redman
New Mexico State University
CTN-4
Mentor: Sam Garcia

Presentation Title: Cryptology

Presentation Abstract: Cryptology is the study of cryptography (encoding & decoding data) and cryptanalysis (analyzing encrypted data to break the codes). There have been many types of encryption techniques used over the centuries from using basic switching of letters in words to very complex mathematical algorithms. My team here at the lab is the COMSEC team, which stands for communication security. Therefore, my goal in doing this research project is to provide a basic understanding to my team of the history of cryptology, defining some terms used in this field, and being able to demonstrate some basic forms of cryptography. This project basically consisted of doing research in the field of cryptology to learn the history of the subject, study math techniques in the field of number theory, and reading textbooks to learn how all different types of logic and mathematical techniques come together to provide data security. Through my research thus far, I have learned that cryptology is an ever growing knowledge since cryptographers have to keep ahead of the cryptanalysists to ensure the security of data being sent over the internet. Also there are too many types of encryption for me to study in one summer so I am only able to research a few types.

Adrian Romero
New Mexico Highlands University
HPC-1
Mentor: Doug Coombs

Presentation Title: LANL HPC Monitoring via Skummee

Presentation Abstract: An enhanced approach of monitoring HPC super computer clusters, which shies away from traditional methods used here at LANL and elsewhere, was brought to the attention of the HPC division due to a tri-lab collaboration between LANL, Sandia, and LLNL to improve tools for monitoring super computer clusters. The challenge of creating a more efficient means of monitoring our HPC systems would essentially boost our ability to understand and resolve problems and our ability to avoid problems before they emerge; reduce our costs by making people more efficient and improve our ability to field increasingly large systems with the same staff. Upon successful completion, system administrators will be provided with an improved integration of the various data types and sources gathered, as well as gaining an opportunity to focus on more vital areas of monitoring since there will be a decrease on the amount of unnecessary troubleshooting. For operators, various opportunities can arise from this as well: an integrated view for all systems, and movement from paper systems to online monitoring via Web/DB systems. Software developed at Lawrence Livermore is the basis for a current and more specialized implementation. Skummee, a package created for monitoring hosts in a large-scale environment, was designed mostly with SNMP in mind. Skummee can and is, however using other means of collecting data. Skummee includes threshold status checking/reporting as well as historical trending. Data is stored in two forms: in MySQL tables, which contain host/variable status; and in Round Robin Database (RRD) files for the historical trending. This allows for quick access to overall machine status (via MySQL) and comprehensive/graphical trending (RRD), both of which have PHP web interfaces. Skummee is designed to execute via cron every five minutes. The RRD files contain three RRA's (Round Robin Archive) which are updated periodically: once every five minutes kept for one week, once an hour kept for one month, and once a day for kept one year.

Ben Santos
New Mexico Highlands University
HPC-1
Mentor: Doug Coombs

Presentation Title: Roadrunner System Monitoring (RASilience + LANLx)

Presentation Abstract: System monitoring is crucial in High Performance Computing. LANL, LLNL, and Sandia are all faced with this common problem and are all addressing it, often in collaboration. As clusters are becoming larger, the volume of data that can be collected continues to grow as well. Early estimates show that Roadrunner will be generating roughly a million messages a week. This introduces a problem for the group of individuals who are analyzing the machines' reliability, accessibility, and serviceability. Not every message generated is of importance to the teams analyzing the data. A single actionable event, such as a reboot on the machine may be represented by several thousand messages. That is too many messages for one individual to sort through to determine that the machine was rebooted. The RASilience system, developed at Sandia National Laboratory, offers many filter techniques to reduce the volume of data that is going to be monitored. A specific functionality is the flexibility to create context correlation filters for data compression. A LANL extension is being developed to extract filter definitions into configuration files; this will provide us with granular permission control on any given data type that is being collected and simplify the filter tuning process. The RASilience system was built on top of a ticketing system that included vital extensions for monitoring large systems such as asset tracking and event tracking. The interface is web-based, but also contains a command line interface as well. It is completely written in Perl and served by Apache Web Server with a back-end data storage currently being driven by a MySQL 5 server. The system is currently in an alpha testing stage and has successfully gathered data from Yellow-Rail and RRZ in a development state. The current LANL process for monitoring system data involves user intervention. We envision this system will ultimately eliminate rigorous manual procedures.

Del Slane
Columbia University
HPC-3
Mentor: Robert Cunningham

Presentation Title: Referential Content Management for Redundant Information

Presentation Abstract: Existing content management systems (CMS) link between articles with ease when in "wiki" format, organize information in hierarchies like with included modules for the open source CMS Drupal. Despite this, none of them create an scheme for content that draws its material from what is already created outside of simply linking to it. Currently the computing.lanl.gov web site contains the same information in many different locations, and hence must be altered in multiple places when a change is necessary. However, with dynamically generated content that simply references "base content" or other compiled articles, there is only one copy of the information--and modifying it changes the viewed data in all articles referencing that base content. Combining this referential, dynamic content generation scheme with a hierarchy for organization as well as keyword tagging/indexing offers a superior experience with this type of web site by offering end users multiple intuitive ways to find the information they are looking for, as well as an elegant system for managing the content.

Jake Stupka
New Mexico State University
NN/N-4
Mentor: Darren Wallace

Presentation Title: Data Management in Google Earth

Presentation Abstract: In order to propagate Los Alamos National Labs' (LANL) international programs collaboration with other countries, the Lab must have an effective way of displaying their developments, as well as prove their usefulness. Through a simple interface between a number of databases and the Google Earth (GE) basic format there is a system that can achieve a number of goals to help LANL's cause. In GE, this approach provides real-time data of equipment that may be in use and provide data visualization of a given area. This is a valuable tool in data management for LANL, it provides an alternative to excel spreadsheets and turns numbers into places. Another effective use of this interface is cutting down on travel costs. Through plugging in the information about equipment that may need to be maintained or updated, and in what country, LANL can collaborate with other national labs in the United States and utilize travelers already in the area to do what needs to be done rather than spending money on travel for that one purpose. This reduction in travel costs can be considerable. This database interface would be accessible to anyone who needs it with proper authorization and authentication, so it could be implemented everywhere.

EARTH & SPACE SCIENCE

Michael Butler
University of Florida
ISR-1
Mentor: Reiner Friendel

Presentation Title: Relativistic Electrons at Geosynchronous Orbit

Presentation Abstract: Understanding the behavior of relativistic electron populations presents an interesting problem whose solution has a variety of applications, ranging from satellite protection to the safety of humans in orbit. We analyze data from LANL's geosynchronous satellites and attempt to determine a relationship between electron flux dropouts to various parameters, including DST and KP, as well as comparing the flux level preceding and following the dropouts. Data is available from 1991 to 2006, covering an entire solar cycle, allowing for comparison between phases. Initial results confirm previous work that the flux levels before and after the dropout are independent of storm activity, or DST (Reeves et al. 2003). In this prior study, storms were identified by the time of minimum DST, whereas in our study we identify them based on the time of the flux dropout. We find that, in the majority (~50%) of cases, the pre-dropout and post-dropout fluxes remain the same within a factor of two, while increases and decreases are observed almost equally in the remaining cases. We also present results of analysis of other energy channels, particularly those which contain the source population of the relativistic electrons. A statistical analysis of the results will be presented, with the hope being a more comprehensive understanding of high energy electron behavior at geosynchronous orbit.

Meredith Curtis
Rochester Institute of Technology
ISR-1
Mentor: Thomas Prettyman

Presentation Abstract: Application of Image Reconstruction Techniques to Mars Neutron Spectroscopy Data

Presentation Title: Data sets collected by the Mars Odyssey Neutron Spectrometer contain artifacts from spatial blurring and noise, which are limiting factors in the interpretation of surface physical properties. The spatial response of the spectrometer is about 10 degrees (full width half maximum) of arc length, making comparisons to and synthesis with higher resolution optical data sets and geological maps challenging. In addition, blurring artifacts can cause significant errors in the derived surface properties. Properties constrained by neutron spectroscopy include the abundance of water equivalent hydrogen (WEH), the column abundance of CO_2 in the seasonal caps, and the abundance of elements such as Fe and Cl, which have large cross sections for thermal neutron absorption. Computer codes were developed to reconstruct maps of the Martian surface with reduced blurring and noise, which can be subjected to geochemical interpretation with greater reliability. Penalty function and iterative deconvolution techniques (Jansson's method) were implemented and compared using simulated and measured data sets. These techniques were applied to global reconstruction of the Mars neutron spectroscopy data set. Both techniques were effective in removing noise without introducing unrealistic oscillations in the reconstructed maps. Results of the study are presented along with implications to Mars science.

Curt Dvonch
James Madison University
EES-2
Mentor: Dubey Manvendra

Presentation Title: Individual Poster Presentation

Presentation Abstract: We are developing a system for measuring diatomic oxygen (O2) and carbon dioxide (CO2) to ultra-precise levels. We expect precision of up to 3 parts per million (ppm) for O2 and 1 ppm for CO2. The system utilizes a Li-Cor LI-7000 CO2/H2O differential gas analyzer and a Sable Systems Oxzilla differential oxygen analyzer. We are assembling the system, writing control and measurement software in LabVIEW, and incorporating the system into a rugged enclosure for placement in the field. The data taken by the system will be primarily used to investigate soil and plant physiology by measuring the Respiratory Quotient, the amount of O2 required for the oxidation of soil and plant organic matter.

Karun Gogna
University of California, Irvine
EES-6
June Fabryka-Martin

Presentation Title: Environmental Fate of the Drilling Product Quik-Foam® in Local Characterization Wells

Presentation Abstract: The complex stratigraphy and the great depth of the water table makes it challenging to drill, install, and develop reliable monitoring wells around the Los Alamos facility. In this geologic setting, it is impossible to drill deep boreholes without using a diversity of drilling products, and yet also difficult to remove all the drilling products from the completed well. Although drillers use biodegradable products, in several cases reducing geochemical conditions have developed in the vicinity of the well screen as residual organic drilling products begin to break down and microbial populations flourish. Over time, metal hydroxide and carbonate minerals near the screen may also undergo dramatic changes. Under such unnatural geochemical conditions, the monitoring well cannot reliably detect the presence or absence of many contaminants even if they were present. Quik-Foam, a high performance foaming agent previously used to drill many LANL wells, contains alcohol ethoxy sulfate (AES) surfactants, which can form micelles in aqueous solution. Some proportion of the micelles, as well as their monomeric constituents, can potentially partition onto rocks or other drilling products and remain in the subsurface, allowing microbial populations to develop over time. The effective critical micelle concentration (CMC) for the surfactants in Quik-Foam will be determined by measuring the change in the fluorescence emission spectrum of pyrene monomers in aqueous solutions. Then batch sorption experiments will be conducted using a total organic carbon (TOC) analyzer to determine whether Quik-Foam sorbs to rocks or other drilling products encountered while drilling. These data will allow for the evaluation of various hypotheses for the mechanisms by which organic drilling fluids may be trapped in the subsurface.

Krista Gray
University of Oregon
EES-2
Mentor: Nate McDowell

Presentation Title: The Response of Understory Vegetation to Pinon Mortality on the Pajarito Plateau.

Presentation Abstract: The recent piñon mortality in the southwestern USA is considered a "canary in the coalmine" of global warming impacts on semi-arid regions. Piñon mortality has resulted in a 70% loss of photosynthetic leaf area on the Pajarito Plateau. This mortality resulted in a significant reduction in ecosystem carbon uptake potential. However, understory vegetation such as grasses and forbs have increased growth after the piñon mortality, which may compensate for the loss of photosynthetic leaf area e.g. ecosystem homeostasis. Our objective was to quantify the response of understory vegetation to piñon mortality and to climate variability. We hypothesized that understory growth will compensate for the loss of piñon leaf area but would remain sensitive to climate. Leaf area has been monitored at TA-51 and at Bandelier National Monument since 1993, allowing examination of the response to drought and piñon mortality. In addition, for 2005-2007 we made measurements of crown area, the approximate ground area a plant covers, and leaf biomass or dry weight bimonthly in transects. Leaf area was then calculated from the harvested vegetation. Understory leaf area has drastically increased since the mortality event in 2002 at both Bandelier and LANL, bringing ecosystem total leaf area to near the same level it was prior to mortality. However, understory leaf area remains sensitive to seasonal and interannual climate variation. We suggest that understory leaf area is a critical homeostatic component of ecosystem carbon and water cycles in this region.

Christian Lucero
New Mexico Institute of Mining and Technology
EES-11
Mentor: Charlotte Rowe

Presentation Title: The recovery of the three-dimensional shear-velocity model from surface-wave dispersion, teleseismic receiver functions, and gravity observations using the LSQR inversion method.

Presentation Abstract: By improving our models of seismic phase propagation through the Earth, we can better predict seismic parameters for events of interest to the nuclear test monitoring community. Most Earth models are derived from a single geophysical parameter and thus are prone to problems arising from ambiguous or sparse data. We are exploring the benefits of inverting multiple geophysical parameters simultaneously to derive a model that fits a variety of observations and is constrained by other parameters where any single data type may be poorly represented. In this project we solve for the seismic shear-wave velocity for a region in China, using surface wave dispersion, teleseismic receiver functions, and gravity observations. The combined large data sets, however, pose difficulties in terms of stability and limited computing resources. Many direct inversion techniques such as singular value decomposition (SVD) are theoretically useful, but computationally impractical for large systems. We have adapted our code instead to use an iterative, LSQR conjugate gradient method. LSQR is particularly useful for solving large, over determined sparse systems using a sparse storage system. Application to our velocity model problem results in a dramatic improvement in both computational time and storage. Storage for our smaller test model consisting of 456 map cells, each having 55 layers has been reduced from 11.6 Gigabytes to only 16.7 Megabytes. We have achieved a 350-fold reduction in run-time, allowing the researcher to repeatedly perform the inversion with different damping and smoothing parameters within an acceptable time frame.

Daniel Romero
New Mexico Insitute of Mining and Technology
ERSS-GS
Mentor: Phil R. Fresques

Presentation Title: Baseline Radionuclide and Nonradionuclide Concentrations in Soils, Vegetation and Small Mammals at the Proposed Expansion Area at TA-54 Area G: 1994-2005

Presentation Abstract: Area G is a 25.5-hectare (63-acre) fenced, low-level radioactive solid waste processing and disposal area located on the east end of Mesa del Buey at Technical Area 54 at Los Alamos National Laboratory (LANL). This disposal area has been in existence since 1957 and is expected to be filled by the year 2015. Thus, a new area, located just west of the Area G site, has been proposed for the expansion of disposal activities. Since 1994, we have been collecting baseline levels of radionuclides and nonradionuclides in soils, vegetation, and small mammals to assess potential impacts at the expanded site once operations begin. Baseline statistical reference levels (mean plus three standard deviations) of radionuclides and nonradionuclides in these media are presented and most compare well with regional background concentrations.

A. C. Schmidt
University of New Mexico
AET-2
Mentor: J. H. Fasel III

Presentation Title: Superluminal Emission Processes as the Key to Understanding Pulsar Radiation

Presentation Abstract: Theoretical and experimental work has established that electromagnetic radiation can be generated by polarization current distributions (rather than, more conventionally, by currents of free charges) and that these radiation sources are, most remarkably, not subject to the universal speed limit. Since 2004, a small team at LANL has conducted analytical, computational and practical studies of radiation sources that exceed the speed of light. These works show that the radiation field generated by a localized charge in superluminal circular motion has the following intrinsic characteristics: (i) It is sharply focused along a rigidly rotating spiral-shaped beam that embodies the cusp of the envelope of the emitted wave fronts. (ii) It consists of either one or three concurrent polarization modes that constitute contributions to the field from differing retarded times. (iii) Two of these modes are comparable in strength at both edges of the signal and dominate over the third everywhere except in the middle of the pulse. (iv) The position angles of each of the dominant modes swing across the beam by as much as 180° and remain approximately orthogonal throughout their excursion across the beam. (v) One of the three modes is highly circularly polarized and differs in its sense of polarization from the other two. The coincidence of these characteristics with those of the radio emission received from pulsars is striking, especially coupled with the experimentally demonstrated fact that the radiation intensity on the cusp decays as $1/R$ instead of $1/R_2$ and is therefore intrinsically bright. Virtually all of the enigmatic features of pulsar radiation can therefore be explained using a single, elegant model with few input parameters and no external assumptions.

Angela Torney
Stanford University
EES-2
Mentor: Nathan McDowell

Presentation Title: Nitrogen, not water, is the dominant driver of mortality in high density ponderosa pine forests

Presentation Abstract: Over the last century in North America, fire suppression has allowed forest density to achieve unprecedented levels, negatively impacting tree growth and survival by increasing inter-tree competition. Forest mortality may also be exacerbated by climate change-associated droughts. In this study, our objective was to examine the impact of competition and drought on tree growth and survival, and our working hypothesis was that water stress is the primary driver of mortality in high density stands. Our field site was located at Monument Canyon Research Natural Area in the Jemez Mountains, and three stands of varying density were compared: a high density stand (H), a stand with low density due to the presence of fire (LF), and a stand with low density due to management thinning (LT). Using wood cores from 10 trees per site, we assessed stomatal conductance via carbon isotope ratios (_13C), and we compared data from time periods before and after fire suppression. If our original hypothesis had been correct, stomatal conductance would have been higher in stand LF than H, but _13C suggested that stomatal conductance was higher in H than LF. A possible explanation for this result was that H was experiencing nitrogen starvation, and this alternative hypothesis was supported by measurements of leaf and soil nitrogen concentrations, both of which were lower in stand H than LF. Results from stand LT are pending. Current results suggest that mortality within high density stands in western North America may be driven by nitrogen starvation rather than water limitation.

ENGINEERING

Benjamin Bachmeier
University of New Mexico
PMT-4
Mentor: William Smith

Presentation Title: Installation of Electromechanical Systems in Glove Boxes

Presentation Abstract: Plutonium is one of the most difficult of all metals to machine precisely, efficiently, and safely. The goal of the Fourth Plutonium Manufacturing Technology (PMT-4) group is to achieve ultimate machining precision of Plutonium, overall efficiency of the process, and safety of Plutonium and its handlers. PMT-4 does this by installing and maintaining the best equipment in the world. Currently the obsolete process is inefficient, not precise enough, and there is overall to much human interaction with the Plutonium. The first project is installing a Precitech Lathe into a glove box and having it ready for operation as soon as possible. One Precitech Lathe has already been installed and is proving to be state of the art. The second project is maintaining and programming a modular trolley system designed for a glove box line by engineers at Los Alamos National Laboratory (LANL). Programming this machine is a priority and writing training/maintenance manuals is a high priority. The third project is a constant, and it is safety. It is the highest of all projects and goals. All the boxes and systems must be ready for installation as soon as possible, and to ensure the safety of the workers and the users the group focuses on anything and everything that could be of harm to either people. By installing state of the art equipment all of goals listed are achieved. With these new systems productivity will increase the already installed system that replaced the obsolete systems. In the end the final product of PMT-4's labor will prove to be the standard and will set the standard much higher.

Marcus Bailon
New Mexico Institute of Mining and Technology
WCM-2
Mentor: Peter Lopez

Presentation Title: Reverse Engineering Laser Alignment System for T-Base Lathe

Presentation Abstract: A T-base Lathe is currently being installed at TA-55 PF-4 and is undergoing extensive engineering review to ensure full capabilities of the machine are met. Currently alignment of Pu parts for the T-base lathe is done utilizing a tripod which is setup outside of the glovebox. Recently the glovebox was retrofitted with a self leveling system (Fabreeka isolation pads) that enables the system to float and isolate itself from the floor of the facility. With a free floating system the floor can no longer be used as a reference for aligning parts. The design improvement will allow the alignment system and glovebox to move as a whole unit making it an integral part of the glovebox. Reverse engineering the existing upper portion of the tripod equipment enabled us to create a conceptual design for the mount. A model was created using WCM-2's capability to produce a quick ceramic based replica of the design, which ensured tolerances and design aspects were met before sending the part for fabrication. Ultimately the final design will be machined and installed onto the glovebox. This will allow the weapons component manufacturing group to achieve one of its programmatic deliverables.

Joe Blaylock
University of New Mexico
PMT-5
Mentor: Paul Moniz

Presentation Title: Controlling Welding Atmosphere to Produce Certified Welds

Presentation Abstract: Since the beginning of the space program, there has existed a need for power and heat on space craft. The decay of Plutonium-238 generates heat that can be used for various tasks like keeping electronics warm in space. Radio thermal generators utilize the unique radio-thermal properties of Plutonium 238 to provide electricity. The encapsulation of Plutonium 238 is done solely at the Los Alamos National Laboratory by the Pu-238 Science and Engineering group. Because of the high activity of Plutonium 238, it is important that it be kept securely inside of its cladding while being transported and during its use to generate heat or electrical power. The Department of Energy has very strict requirements regarding the encapsulation of Plutonium-238. The welds that seal the capsules must be very precise, and nearly flawless. Obtaining this degree of perfection requires state of the art welding equipment as well as a very inert welding environment. The welding is done inside a glove box designed to maintain a helium atmosphere. To certify the integrity of the weld, non-destructive testing is performed. This insures the laboratory reached the level of quality and safety required by customers like NASA.

Justin Bowyer
New Mexico State University
AOT-MDE
Mentor: Tajima Tsuyoshi

Presentation Title: Development of Temperature-Mapping Systems for 1.3GHZ-9

Presentation: Abstract: The mapping of outer wall temperature during the vertical test of a superconducting radio-frequency (SRF) cavity has been one of the most useful tools to detect bad spots of the cavity. However, few systems except a rotating-arm type one have been developed so far for 9-cell cavities. Since it will be an essential tool to identify the failure of the cavities, we started to develop a fixed-board-type temperature mapping system that will enable us to map the temperature of 9-cell cavities in a much shorter time than rotating-arm type. This paper describes the design, status of the development and preliminary tests of the design.

John Brooks
University of New Mexico
Armando Martinez
New Mexico State University
HX-6
Mentor: Renee Ortiz

Presentation Title: Fast Closing Valve Timing Analysis

Presentation Abstract: The Dual Axis Radiographic Hydrodynamic Test facility is LANL's answer to all the nuclear watchdogs cries to be environmentally friendly. It satisfies the need for maintaining the stockpile stewardship program while minimizing potentially hazardous effects that underground/outdoor testing may cause. When engineering something of this magnitude, modifications to pre-existing systems is inevitable as time goes on and technology evolves. Even though this project has been in the works for the last 15+ years, there are always modifications and upgrades that need to be made to pre-existing systems, or have new systems developed to solve whatever the current crisis of the time is. Enter the Fast Valve at DARHT. Picture a beautiful beam channeling down the accelerator hall. Countless man hours have gone into steering the beam down to its intended destination, but accidents happen. It would be disastrous if the beam hit the side of the accelerator cell walls. Or, if after hitting the target a beryllium window was broken out. The cost incurred of an incident like this happening is unfathomable. The entire accelerator would have to be stripped apart, cleaned, and reinstalled. This process would literally take years and tens of thousands of man hours to repair. We have come up with a solution to protect everything upstream (inside the "protective envelope") in the event of such an incident. It is called the Fast Valve. Its primary duty is to open and close before and after each shot. In normal operation, its opening time is somewhere around 7 seconds. Closing the valve on the other hand is a little faster with a nominal closing time of 23 milliseconds including electrical hardware. Our intent was to show that by building an in-house setup, we could cut the closing time in half compared to the manufactures provided system.

Marcus Cappiello
Los Alamos High School
MST-8
Mentor: Stuart A. Maloy

Presentation Title: The Effects of Large Scale Plastic Deformation on Microstructural Development in HT-9

Presentation Abstract: There are many methods available to plastically deform a material to obtain desired mechanical material properties. These methods include Equal Channel Angular Pressing (ECAP) and rolling, as well as others. In the ECAP method, the sample to be deformed is first embedded in another container material such as nickel. This sample is then deformed through a 90 degrees bend several times. In rolling, the material sample is drawn through two rollers at a temperature below its recrystallization temperature compressing the material into a sheet. The ECAP method was performed on alloy HT-9 (9Cr-1Mo, ferritic-martinsitic). The rolling was done on HT-9 to a finished product of 3mm and 1mm thickness. These samples were viewed under a high power optical microscope to observe microstructural differences between the samples. The analysis shows that the grain structures in the rolled and ECAP'ed samples were smaller and more compact as compared to the as cast material which showed randomly oriented large grains. The difference between the rolled HT-9 and the ECAP'ed HT-9 is still under review and will be resolved by the Student symposium. Hardness tests were also performed to determine the effects that these processing steps had on the mechanical properties.

Ben Clay
Virginia Tech
ADTSC CCS-3
Mentor: Sami Ayyorgun

Presentation Title: Stochastic Rate Control in Video Streaming

Presentation Abstract: Queuing theory and buffer control are areas of great interest as networks become large and unmanageable. Specifically, guaranteeing a quality of service (QoS) in a large, uncontrolled network such as the internet is important from both a business perspective (selling a service at a specified QoS) and a user's perspective. In order ensure that data reaches the intended target at the intended rate, stochastic rate control algorithms can be used to guarantee a service within a given probability. To this end, previous work has determined and elaborated upon mathematical methods to achieve optimum buffer control given a generic packet-based data source. Our work intends to extend these algorithms to streaming video, using subjective analysis to determine the appropriate equations and values to make the rate control transparent to the end user. To do so, a server-client implementation has been built on top of the popular open-source video player VLC. The rate control algorithms specified in previous work are built as the core of the server application. The client code "tricks" VLC into thinking its content is coming from a local disk, simplifying the overall implementation and keeping VLC as close to its intended purpose as possible. Preliminary results suggest that rate control in video at a byte level could potentially be used to improve subjective measures of quality from a user's perspective. However, further exploration of specific cumulative distribution functions needs to be completed before conclusions can be drawn.

Paul Day
Stanford University
PMT-4
Stuart Rector
New Mexico State University
AET-5
Mentor: Cameron Turner

Presentation Title: Robotic Automation of Plutonium Oxide Packaging

Presentation Abstract: Robotic automation of glovebox contained manipulation of fissile material is highly desirable due to the hazards involved in performing such tasks by hand. It is desired to package plutonium oxide in robotically sealed cans to reduce risk to LANL workers. Due to the nature of the material being handled, it is imperative that the robotic systems reliability be excellent, necessitating a comprehensive battery of testing. A robotic test bed was developed in a non-hazardous, unclassified environment in order to determine the systems reliability. Test runs were performed using each of two can geometries scheduled for use in the real system: the ARIES Convenience Can and the newer COGEMA can. Each can was put through a round of 340 process cycles, each of which consisted of two separate can movements for a total of 680 can handles per round. Any mishandling of the can resulting in a can drop or release failure by the robot was considered a handling failure. At the end of the testing period, the system performed without a single failure for each of the can geometries. From this data, we can say with 99.9% certainty that the handling failure level will be less than 2 per 100 runs of the system. These results are extremely valuable in that operators can be confident that the system will perform with a near perfect operating record for the duration of its use.

Paul Gibbs
Colorado School of Mines
MST-6
Mentor: Deniece Korzekwa

Presentation Title: The Straight and Narrow: Computer Modeling of casting For GNEP

Presentation Abstract: Recently there has been a push to advance the development of nuclear reactor fuels to be more efficient and produce less waste. One of the goals of the Global Nuclear Energy Partnership (GNEP) is to develop processing methods that reduce contaminated waste generation during the fabrication of fuel assemblies. This project focuses on the feasibility of gravity casting uranium alloy rods into reusable graphite molds to replace the current production method of semi-pressure casting into single use quartz molds. The new production method is intended to produce higher quality rods with less contaminated waste generation. These rods pose a particular challenge to cast because they have a very high length to diameter ratio, the computer models are 350 mm long and have a diameter of 4 mm. These dimensions restrict fluid flow into the mold cavity and cause the mold to not fill completely. Computer modeling is being used to develop the mold design and casting process conditions in preparation for future experimental test castings. The modeling was preformed using the Truchas code, a manufacturing simulation tool developed at LANL. The goal, of the modeling project, is to explore what conditions are most likely to result in a successful part without the expense of an experimental casting. To date the project is beginning to yield results, showing that it may be possible to produce acceptable parts, through proper temperature management during casting.

Oscar Gonzalez
New Mexico State University
WCM-1
Mentors: Peter Lopez & Dave Gubernatis

Presentation Title: Tool Insert Development for Machining Plutonium

Presentation Abstract: Los Alamos has a rich history in the design of nuclear weapons. One of the lab's current missions is nuclear stewardship. LANL must develop and maintain the capability to manufacture all pits on the enduring nuclear weapon stockpile at TA-55. In order to manufacture pits, Pu must be refined, casted and machined. One way to modernize and improve machining operations one must look to maximize insert tool efficiency. Current tool inserts are made out of tungsten carbide (WC). We plan to compare modern tool coatings to the current insert. All machining variables such as feed rate and feed speed will be constant and our only variable will be our insert coating. Several coatings were selected for this project. These include: cubic boron nitride, titanium diboride, tungsten carbide alloy, titanium nitride and poly-crystalline diamond. Test pieces will be manufactured of the following metals: stainless steel, aluminum, cast iron, copper and nickel. These test pieces and inserts will be analyzed using optical profilometry, surface finish gauges, high speed camera, infrared camera and surface comparator. The insert that shows the exhibits the best performance will be recommended to cut a Pu test part not a surrogate.

Jorge Guerra
New Mexico State University
INP-SMS
Mentor: Mark Dinehart

Presentation Title: Wet Vacuum Design in the Chemistry and Metallurgy Research Replacement's Nuclear Facility

Presentation Abstract: The Chemistry and Metallurgy Research building (CMR) is a 550,000 square foot building constructed at Los Alamos National Laboratory (LANL) between 1949 and 1952. The CMR building currently houses mission critical analytical chemistry, materials characterization, and actinide research and development capabilities. These capabilities support the National Nuclear Security Agency (NNSA) stockpile stewardship missions as well as programs within Nuclear Nonproliferation, Nuclear Energy, and Environmental Management. The current Risk Management Strategy for the CMR facility commits NNSA and LANL to manage the facility to a planned end-of-life on or about the year 2010. The Chemistry and Metallurgy Research Replacement Project is tasked to relocate and consolidate mission-critical capabilities associated with the existing CMR Facility. Two facilities are currently being planned, the first, a Radiological Laboratory, the second, a Hazard Category II and Security Category I Nuclear Facility. The design/build contract for the Radiological Laboratory has been awarded and the contractor is currently finalizing the design of the building. The Nuclear Facility and associated SFE in the final stages of preliminary design phase. A detailed engineering design review of the wet vacuum systems in both the Radiological Laboratory and the Nuclear Facility were requested to address problems with operability, reliability and maintainability for similar systems in the TA-55 Plutonium Facility. In addition, the project requested an analysis of the information needed to progress the designs from preliminary to final. The design review involved a comprehensive evaluation of the engineering basis for the wet vacuum systems including a review of the functional and operational requirements, system design descriptions, piping and instrumentation diagrams, sequence of operations and 3-D models. Lessons-learned from the operating organizations at the Laboratory were also developed for this system and will provide a basis for much of the design input to the architectural engineering firms. The design review comments have been generated and will be forwarded to the project team and the architectural engineering firms responsible for the designs. Significant changes to the preliminary designs are anticipated based on the results of this review including modifications to the piping design, criticality geometries, and safety basis assumptions.

Chris Hammetter
University of California, Santa Barbara
IMMS
Mentor: Matt Lewis

Presentation Title: Probing Elastomer Foams with Dielectric Elastomer Devices

Presentation Abstract: The mechanical behavior of elastomeric foams can be extremely complex and very difficult to model or predict. Of particular interest here are the effects of aging on the mechanical performance of the foam. The foams of interest have shown that their ability to support loads is diminished over time when stored in compression. When the cushioning ability of the foam is critical to a system's performance, this creates questions about that system's lifetime. Current methods for determining the condition of the elastomer foams require that samples of the foam be removed from the system and tested. This can be very costly and it appears that the very act of removing the foam may prevent accurate measurement of how the foam will behave in place. There is a need for an embeddable device that can monitor the state of the foam without significantly affecting the performance of the foam. This presents an interesting technical challenge in several respects. Firstly, the foam's aging and positioning is such that the foam's stiffness decreases without any change in macroscopic strain. Thus, a sensor is required that can probe the stiffness of the material without the use of the initially induced strain. Secondly, the strains over which the foam must perform are quite large, up to 60%. Luckily, a promising solution exists through the use of dielectric elastomers. Dielectric elastomers offer the ability to create actuators and sensors that are capable of these large strains while also having properties of the foam-forming elastomer; thus offering good compatibility and negligible effects on the performance of the foam. The purpose of this presentation will be to further describe the performance concerns of the elastomer foams, the fundamentals of dielectric elastomer actuators/sensors, and the possible designs of an embeddable device.

Richard D. Herrera
University of New Mexico
PMT-4
Mentor: Jerry Lugo

Presentation Title: Interference of the 40mm Gas Gun Surrogate Samples

Presentation Abstract: As a summer student Richard Herrera will be mentored to develop the test Interference of the 40mm Gas Gun surrogate samples. Work includes the following: Geometric Dimensioning and Tolerancing, blueprints and determining the tolerance of a given machined specimens. He will be using AutoCAD, data entry, experimental design, development of test parameters, usage of Code and Standards such as the American Society of Non-Destructive Testing (ASNT), American Society of Mechanical Engineers (ASME), and the National Institute of Standards and Technology (NIST). This work will include the use of hand held measuring tools, such as micrometers and dial calipers. We will be conducting measurements in the 0.0001" range. Also, he will be trained to use a sophisticated computerized measuring instrument called "Optical Gauging Product Smart-Scope. The student will work at TA-35 in a non-cleared area. This facility houses the equipment for all PMT-4 cold machining operations.

Fawn Hornsby
North Carolina State University
D-3
Mentor: Michael Brown

Presentation Title: An Assessment of the QUIC Dispersion Modeling System for Flow Around Isolated Buildings

Presentation Abstract: Fast-response transport and dispersion modeling of airborne toxics plays an important role in national security—in particular, this includes emergency response, training and planning, as well as vulnerability assessments. The Quick Urban and Industrial Complex (QUIC) dispersion modeling system was created in order to help assess the consequences of chemical, biological, or radiological airborne releases in cities. QUIC explicitly accounts for buildings, but is faster than traditional computational fluid dynamics models. Based on a dissertation by Röckle (1990), this model computes three-dimensional winds around buildings using diagnostic and empirical methods as well as mass conservation. In this summer project, model output was compared to wind tunnel data from experiments conducted at the USEPA in order to determine the accuracy of the model and to possibly improve the empirical algorithms. In particular, a careful evaluation of the cavity lengths of rectangular "buildings" at off-angled winds revealed the need for new parameterizations. Changing the formula for the effective building width and moving the starting point for the cavity length formed a more accurate picture of the wind vectors. Most importantly, these advances will lead to improved CBR transport and dispersion calculations under a wide variety of wind conditions.

Robert Igel
Bradley University
D-5
Mentor: David DeCroix

Presentation Title: Modeling of an Aerosol Collection Inlet for Interior Monitoring

Presentation Abstract: The dispersion of biological agents into populated environments is a serious terrorist threat faced by the United States. Possible targets of biological terrorism include densely populated areas such as stadiums and public transportation systems. Los Alamos National Laboratory wants to be able to collect air samples in these areas using an aerosol inlet for a collection device that has been designed to be installed in the HVAC system of densely-populated buildings. The inlet was designed to collect particles less than 10μm. Preliminary testing has been performed on this design; however, a more complete understanding of the inlet is desired. The purpose of this research was to model the same inlet using the Fluent computational fluid dynamics solver to provide more conclusive collection efficiency results and determine the flow characteristics caused by the inlet. The 3-D model of the design, its mesh, and its boundary conditions were constructed in Gambit. This file was then exported into the Fluent solver, where flow conditions – turbulence, flow rate, and particulate size – were specified. Several trials were run varying the flow rate between 2- and 8km/hr and particulate size values of 8-, 12-, and 20μm. The anticipated results of these trials are that the inlet will collect the vast majority of the 8-μm particles, only a small percentage of the 12-μm particles, and none of the 20-μm particles. However, more simulations must be run to determine the streamlines and other flow properties of the inlet's geometry and its overall efficiency. The results from this research will better enable the detection of biological agents harmful to building occupants.

Matt Jackson
University of New Mexico
PMT
Wolfgang Dworzak

Presentation Title: 3013 Headspace Gas Sampling Project

Presentation Abstract: This project began with the need to analyze the gas composition of a single 3013 can (MIS-STD-1). The objective was to design, develop, cold test and install a can punch/gas sampling system within the confines of a glovebox in PF-4. The said can punch should also be capable of taking samples of other LANL type, as well as Hanford type cans. Our design concept was to use a small drill press in order to penetrate both the outer BNFL can, the inner 3013 can, and convenience can sequentially. We designed a plate that fits on the top surface of the BNFL can and equipped it with an o-ring to seal the plate with the can. We then had a Hot Tap Tool fillet welded on the top of that plate. The drill bit itself passes through this Hot Tap tool and is able to contain pressures of up to 265 PSI while the drill press is operating. Once a can layer is punctured the contained gas is expanded into an evacuated manifold where a pressure reading can be taken, followed by a sample of that expanded gas. This entire system, part by part, was modeled using SOLIDWorks software. These drawings are a vital part of the design sequence and would also be used in creating the DCP package witch will enable the installation of this project into GB-154. Currently the design is near completion of the Cold Testing Phase. It is set up and operational in a cold lab at TA-55. Vacuum, Pressure, and leak tests have been performed on the Can Punch setup, as well as drill tests which simulate the actual anticipated operating sequences. The DCP has undergone a 60%, 90%, and a 100% review meaning once our cold testing is complete installation of the project into GB-154 can begin.

Salomon Jimenez-Zapata
University of California, Santa Barbara
IMMS
Mentor: Matt Lewis

Presentation Title: Finite element simulation of electro active polymers

Presentation Abstract: Electro active polymers are materials that respond to electromechanical stimulation and are capable of sustain very large elastic deformations (up to 700%). Electrostatic attraction forces between charges in the material generate stresses; the form of these stresses is dictated by the constitutive law and cannot be assumed to have any other form. The free energy density for a dielectric material exhibiting rubber like elastic behavior and constant dielectric properties is proposed; and the total true stress (that is the stress due to mechanic and electrostatic loading) is determined by the constitutive equations. The virtual work exerted on the material by external agencies such as surface tractions and electric charges, is translated into a finite element scheme for large deformations. Using this formulation we developed a custom stand alone finite element program to simulate the behavior of electro active polymers under conditions of plane strain and plane electric fields.

Tyler Karrels
University of Wisconsin, Madison
ADTSC CCS3
Mentor: Sami Ayyorgun

Presentation Title: Improving Network Connectivity in Wireless Ad Hoc Networks

Presentation Abstract: TCP/IP routing is the standard for static wired networks, but TCP/IP cannot quickly adjust to changes in network topology that can occur in wireless ad hoc networks. A wireless ad hoc network's topology is dynamic because hosts eventually lose power, hosts' transmission ranges may vary over time, hosts may become damaged, or hosts may enter or exit the network's transmission range. These problems require new routing paths to be established to maintain network connectivity. The purpose of our research at Los Alamos National Lab (LANL) is to improve, or at least maintain, connectivity between hosts even when the network topology is drastically altered. We propose a new routing protocol based on the BitTorrent (BT) algorithm that creates multiple paths to the network sink and monitors these paths to decide which is optimal. Network simulations have been conducted in Matlab using a simulator developed for this research. For a comparison to existing routing algorithms, Dynamic Source (DSR) and Load Balance (LB) routing algorithms have been implemented in addition to BT routing. Simulations are being run with networks of varying size and topology. The three topologies used are grid, random, and degree based. Preliminary results for small networks have shown that DSR and LB algorithms perform similarly with a grid network topology and no node failures. After implementing node failures, it is expected that BT routing will be more resilient by quickly repairing routes. It is also expected that BT routing will establish quicker routes even when a network is heavily loaded.

David Limmer
New Mexico Institute of Mining and Technology
W-7
Mentor: Michael Smith

Presentation Title: Determination of the Hydrogen Concentration Distribution around a Crack Tip Using Numerical Analysis

Presentation Abstract: Quantification of the hydrogen concentration distribution around a crack tip in embrittled steels are complicated due to interstitial diffusion and accompanying low concentrations. At present, an experiment has been proposed in which a pre-cracked sample will be charged with hydrogen, and cut into a series of cubes to act as a grid. These cubes will then be analyzed for their respective hydrogen content and a map of the concentration distribution will be developed. This study looks at the feasibility of such an experiment by attempting to quantify the hydrogen losses due to the processing required. Using the the finite element analysis (FEA) software, Abaqus, we have developed a coupled deformation-diffusion and pseudo-coupled diffusion-heat transfer model to predict the amount of hydrogen out-gassing after charging, during machining, and through a proposed storage time. A variety of situations were studied in order to recommend a process which minimizes loses. The amount of hydrogen lost was calculated for each situation and the feasibility conditions for the experiment were determined.

James Lischeske
University of California, Davis
WT-6
Mentor: Kevin Hase

Presentation Title: Dynamics in Granular and Micro-Fluidic Flow

Presentation Abstract: Continuum fluid dynamics has proven to be an incredibly useful tool over the past two and a half centuries in describing fluid systems. However, when the length scales of the flowing systems are such that the continuum hypothesis no longer applies, the direct application of the equations of motion produce a physical results. This study uses a combination of experimental results and molecular and granular dynamics simulations to explore the dynamics of granular flow and micro-fluidic flow, where the relationships and equations of classical fluid dynamics begin to break down. In granular flow, we investigate spontaneous axial segregation in a rotating cylinder by experiment and simulation. We also explore the problem of low-Reynolds Number flow near a solid boundary, where an object falling through viscous fluid approaches the bottom of the container, experiencing forces other than what are predicted by Stokes law.

Jacquelyn Lopez
University of New Mexico
PMT-2
Mentor: Anthony Lupinetti

Presentation Title: Liquid-Liquid Extraction of Iron (III) from Hydrochloric acid solution by Dodecane. Tri-n-butyl Phosphate and Decanol

Presentation Abstract: Liquid-liquid extraction is used to separate plutonium from acidic solutions. Currently, the separating agent used is a 70-20-10% mixture of dodecane, tri-n-butyl phosphate (TBP), and decanol, respectively. TBP acts as the extractant while decanol is a modifier and dodecane is the dilutant. Separations were done by extracting ferric chloride from an HCl solution using organic mixtures with varying amounts of TBP and dodecane. Ferric chloride was used as a surrogate for plutonium to determine the distribution ratio of the system at 25°, 27°, and 29°C, versus the concentration of TBP and HCl to better understand the separation chemistry.

Jessica Maestas
University of New Mexico
DE-9
Mentor: Darcie Koller

Presentation Title: A High Pressure Gas Transfer System for the Operation of a Single Stage Light Gas Gun

Presentation Abstract: The pop gun, located in Ancho Canyon, is a single stage light gas gun that uses helium gas to accelerate a projectile to velocities ranging from 150 m/s to 800 m/s. This is accomplished by pressurizing the breech to pressures of 5000 psi. A projectile is used as a seal between the high pressure breech and the evacuated gun barrel and is held in place by a threaded rod attached to a motor. When the motor turns the threaded rod back out of the projectile it is accelerated down the gun barrel by the high pressure gas from the breech. This system was built in the 1950's and was last upgraded in 1968. Therefore, to improve safety and efficiency during experimentation, remote operation and computer control has been implemented. Implementation of computer control required the upgrade of the gas transfer system to use remotely actuated valves to provide a remote firing capability. The design presented here, gives the details pertaining to the high pressure gas manifold system, the gas transfer and boost system, and the vacuum system. The design of this system consisted of creating a drawing as well as researching and determining what parts should be included and where they should be placed. These parts included remotely actuated high pressure valves, vacuum valves, relief valves, needle valves, high pressure tubing and fittings, and pressure transducers. All parts were purchased and the new system was assembled and prepared for integration with the computer control system.

Ray Martinez
University of New Mexico
WCM-2
Mentor: Peter Lopez

Presentation Title: Automation of Mechanical Systems

Presentation Abstract: Current events within the plutonium facility have offered the expansion of automation verses labor intensive glove box work. A dividing head is a piece of equipment currently used as a precision worm wheel and crank attached to the worm shaft, which is used on a Computer Numeric Control Mill (CNC) to hold stationary parts. Currently, plutonium purification workers do not have an automated system; therefore, everything must be done manually in the glove box, which is very labor intensive. The purpose of this project is to aid plutonium purification workers in holding and rotating furnace tubes and additionally ancillary equipment. To accomplish this task and meet the mechanical system requirements for the dividing head, research on motor capabilities and hands on work with a mechanical designer will ensure that all modifications are captured first through a design drawing followed by the actual installation of the motor. The results expected from this process are a complete design implementation of a motor to the dividing head. Ultimately, automating this process will allow workers to shorten process time in the glove box and reduce ALARA.

Rebecca M. Martinez
University of New Mexico
INP-SMS
Mentor: Tom Gunderson

Presentation Title: Seismic Qualification of Gloveboxes

Presentation Abstract: The purpose of the Chemistry and Metallurgy Research Replacement (CMRR) project is to relocate services performed at the CMR building to a new set of facilities that will include a Radiological Laboratory Utility and Office Building (RLUOB) and a nuclear facility. The new buildings will contain special facility equipment (SFE) that must be seismically qualified to protect the public, the environment and worker safety if a seismic event were to occur. Department of Energy (DOE) codes and standards require SFE to be qualified to a more stringent standard for the nuclear facility due to the nature of the building and the level of hazards involved in running such a facility. To minimize cost and maximize efficiency, gloveboxes to be placed in the RLUOB will be qualified to the same standard as those to be used in the nuclear facility. To help ensure that gloveboxes meet seismic qualification for both facilities, DOE standards and codes for qualification were reviewed, acceptable methods of testing were identified, and a seismic test plan will be proposed for future seismic testing. Following a documentation of standards to be met for qualification and an investigation of appropriate testing methods, a test and test plan will be submitted for evaluation and comparison against other suggested approaches. A final, approved test plan can then be used for seismic qualification of gloveboxes for both the RLUOB and the nuclear facility.

Ricardo Martinez
University of New Mexico
AET-1
Michael Unzueta
University of New Mexico
Reese Myers
Texas A&M
AET-5
Mentor: James Jurney

Presentation Title: Refurbishment of the Bell Jar Assembly

Presentation Abstract: A bell jar is an assembly used to contain an induction heating unit that melts metals. The bell Jar in our facility had not been used in several years so it was in desperate need of a rebuild. The hoses that were on it were corroded, cracking, and outdated. The structure itself needed to be fitted with a new hoist mechanism to lift the top half of the bell jar while at the same time insuring structural integrity. Also, the inside of the bell jar needed to be cleaned and free of contaminants that could cause problems during operations. So, the first step to the rebuild was fitting a hoist and reinforcing the top of the bell jar to support the weight and also provide enough clearance to get materials in and out. The design was sent to a Mechanical Engineer for a computer simulated stress analysis. Step two in the rebuild was getting all the out dated hoses replaced. The hoses were replaced by hoses that underwent an Engineering Equivalency process. Lastly, lifting the lid and cleaning the inside of the bell jar was done using Acetone first to remove oils such as those from fingerprints and then cleaned with Isopropyl Alcohol to remove any excess moisture. The outcome of this project is an updated bell jar that is ready for successful operation.

Aaron Mason
Brigham Young University
DE-6
Mentor: Bryce Tappan

Presentation Title: The use of Bis(triaminoguanidinium) 5,5'- Azotetrazolate (TAGzT) as a Burning Rate Modifier

Presentation Abstract: The high nitrogen/high hydrogen compound, bis(triaminoguanidinium) 5,5'-azotetrazolate (TAGzT) is being investigated for use as a burning rate modifier in nitramine gun propellant formulations. In order to determine the interactions of TAGzT and RDX in combustion, formulations were produced of the two materials at various percent weight compositions and burning rates of the pressed materials were performed. It was found that the burning rate of the mixtures of TAGzT with RDX is greater than the weighted average of burning rates of the individual materials. Gas-phase CHEMKIN calculations were performed on this system and indicated a synergistic affect between the reaction products of TAGzT and RDX yielding some explanation in the observed phenomenology. Gas-phase CHEMKIN calculations on similar systems replacing TAGzT with 3,6-bis-(1H-1,2,3,4-tetrazol-5-ylamino)-stetrazine (BTATz) and N-oxides of 3,3'-azobis(6-amino-1,2,4,5-tetrazine) (DAATO3.5) indicate no such synergistic reactions. The combustion behaviors of these formulations with other high-nitrogen energetic materials as well as pure nitramines will be discussed. Use of the material TAGzT in thermobaric explosives are also discussed and results from air-blast testing of TAGzT based explosives are compared with Composition C4 (90% RDX/plastic binder) and other thermobaric explosives. The air-blast test show that TAGzT based explosives have peak pressures and impulses comparable to C4, however the after-burn of the TAGzT based explosives are much longer and produce more heat than C4's after-burn.

Jason Miles
Montana State University
PM-DO
Mentor: Gerard Montoya

Presentation Title: Glove box Tools

Presentation Abstract: Current Glove box tools need drastic improvements. The tools are very crude and simplistic and as result the glove box workers are injuring themselves; injuries that could be prevented by a simple redesign of the tools used. It was observed that major strains were being placed on the bodies of the workers during unloading of 55 gallon drums. Workers requested that a tool be built that could remove bags and other debris from the drums. To correctly define the scope of the problem the specific glove box being used in TA-50 was observed and it was determined that a gripping tool with a telescoping handle was needed. A preliminary tool design was then modeled in Pro-E, keeping in mind glove box ergonomic design constraints. The model was then redesigned reviewed by CINDY LAWTON who specializes in glove box ergonomics. Currently the tool is still being redesigned with help from GERARD MONTOYA we hope to create a scale model of the tool before the symposium

Kirsten Mourant
University of New Mexico
AET-2
Mentor: Tom Farish

Presentation Title: High Level Systems Model of GNEP Fuel Cycle

Presentation Abstract: A dynamic system model of the Global Nuclear Energy Partnership (GNEP) fuel cycle is being developed using the simulation software Extend. GNEP aims to improve the use of nuclear energy around the world by minimizing waste, maximizing resources and reducing the risk of proliferation. Systems analysis is guiding the decision-making process by allowing researchers to estimate the total system impact of different fuel-cycle decisions over a 50-year period. The model incorporates the major parts of the GNEP fuel cycle including uranium mining, burnup in conventional nuclear power plants, Urex reprocessing, and the subsequent burnup of reprocessed fuel in an advanced reactor. The holistic approach includes a wide variety of metrics such as the cost and quantity of electricity being generated, the quantity of raw materials consumed under different scenarios, the volume of waste, and the radioactivity of waste. The model also tracks certain elements including uranium, plutonium, certain fission products and actinides as the material works its way through the system.

Hailey Murdock
University of Nevada, Reno
AET-3
Stephen N. Paglieri

Presentation Title: 3He Permeation through Fused Silica Inertial Confinement Fusion Targets

Presentation Abstract: Research is currently being done to demonstrate the feasibility of harnessing energy from deuterium-tritium (DT) fusion to produce electrical power. One technology being studied is inertial confinement fusion (ICF). In the ICF approach lasers are used to rapidly compress and confine DT to high temperatures and pressures needed to initiate the fusion reaction. An important issue for ICF research is how helium-3 (3He), the tritium decay product, influences DT fusion. To study this issue laser fusion experiments are being conducted at The University of Rochester Laboratory for Laser Energetics (LLE) OMEGA Laser. Small glass (SiO2) spheres (1100 μm diameter) were initially filled with 5.1 atm by permeation at 220°C, at the Weapons Engineering Tritium Facility (WETF). After the DT filling, each target was filled at room temperature with 3He; helium has a much larger permeability through SiO2 than hydrogen. A filled target was then placed in a manifold with 7.4 cc volume. The permeation of helium out of the target was determined by measuring the rate of pressure rise in this volume. From this data, the permeation rate was determined by simultaneously solving two differential equations. The targets were then sent to the OMEGA Laser, where they were re-loaded with 3He. By recording the time it took to handle and mount the targets into the OMEGA Laser chamber until the laser was fired, the final 3He pressure in the targets at shot time was calculated. The targets were imploded using the OMEGA Laser; the fusion yield from implosion was measured. Experiments with targets at OMEGA provided data on the physics of 3He influence on DT fusion in high temperature plasmas. Preliminary results indicated 3He had a substantial but reproducible and quantifiable effect on fusion.

Michael Nelson
Rice University
AET-1
Mentor: Curtt Ammerman

Presentation Title: Designing a Prototype Heat Exchanger for use in the LANSCE MTS Program

Presentation Abstract: Current U.S. knowledge in the area of advanced, or fast, reactors is limited. Although no fast reactors exist in the U.S., the proton accelerator at LANSCE can be used to bombard test nuclear fuel rods with high fluxes of neutrons to simulate fast reactor conditions. Large amounts of heat are produced in the target assembly when the proton beam strikes it and in the nuclear fuel rods. The purpose of this project was to design a heat exchanger that can not only fit on a Materials Test Station (MTS) target and fuel rod assembly but also remove enough heat to make proposed MTS experiments feasible. Liquid lead-bismuth eutectic (LBE) was chosen as the coolant because of its ability to transfer heat well at a low flow velocity. A shell-and-tube heat exchanger was designed with LBE flowing through the shell portion; water flows up in an annulus between nested tubes and then down through the inside tube, taking heat from the LBE. Between the water and the flowing LBE is another annulus with static LBE contained within an outer tube. This serves to vary the overall heat transfer coefficient and prevents the flowing LBE from freezing. A tank was designed to contain this static LBE, withstand a pressure of 50 psi at 500 C, and allow for complete emptying of the static LBE annuli in less than five seconds. The commercial finite element analysis code ANSYS was then used to determine heat transfer coefficients for the heat exchanger and to determine mechanical strain placed on the LBE drain tank by pressure and thermal expansion. We expect the results to show that the heat exchanger and its secondary parts do not allow excess heat to build up in either the beam target or the fuel rod assembly and are able to withstand the conditions in the LANSCE beam. This project will allow LANSCE to be able to test advanced reactor nuclear fuel rods, which represents a partial solution to the issue of radioactive waste in the U.S. because fast reactors can run on plutonium fuel, reducing the nation's stockpile of waste while also producing electricity.

Blaise Paul
Louisiana State University (LSU)
W-6:
Mentor: Nathan Burnside

Presentation Title:Gas Dynamics Modeling for Pyrotechnically/Explosively Actuated Devices

Presentation Abstract: Pyrotechnically and explosively actuated devices exist in diverse applications where dependability and performance is of the utmost importance. These devices reliably and safely deliver high power in remote locations by converting chemical potential energy into useful mechanical work by means of the gas products produced from combustion. Pin pullers, valves, thrusters, and cable cutters are only a few examples of these devices that carry out critical functions such as parachute deployment, fuel/engine shutoff, and emergency jettison. In the past, empirical data has been the primary means of measuring a devices' performance. Although these experiments are necessary to observe actual device behavior, computational modeling can be implemented to validate the experimental results, and to assist the design process which saves both time and money. The presented work includes numerical predictions for an unsteady compressible fluid flow system, as in pyrotechnically and explosively actuated devices. This is accomplished by solving the governing gas dynamic equations with a high-resolution central scheme technique. The primary goal of this work is to understand performance variations due to the unsteady flow effects for devices with a function time within the same order of magnitude as the gas products acoustic timescale. In the developed one-dimensional model, waves are tracked as they propagate and reflect within the device, and their influence on the solid energetics' pressure dependant combustion is identified. The numerically predicted results are validated by making comparisons to pressurized gas driver experiments, and empirical data obtained from explosive actuators.

Scott Reckinger
Universtiy of Colorado
CCS-2
Mentor: Daniel Livescu

Presentation Title: Application of the Dynamically Adaptive Wavelet Collocation Method to Direct Numerical Simulation of Compressible Turbulent Mixing

Presentation Abstract: In order to push the limits of current numerical simulations for many fluid systems involving multiscale phenomena, such as turbulence mixing, the application of adaptive methods is a promising approach. However, additional constraints on the numerical method, such as accurate solution of all scales ofmotion and minimized numerical dissipation, are required to make it appropriateas a Direct Numerical Simulation method and rule out most AMR techniques. The Dynamically Adaptive Wavelet Collocation (DAWC) method utilizes the localized nature of the wavelet representation to create an adaptive mesh over which to perform computations. The adaptive mesh wavelet-based method allows for higherresolution computation in regions with small-scale turbulent structures, while computing at lower resolutions in areas where only large-scale structures are present, at the same time ensuring effective error control. This ensures that resources are used most efficiently while maintaining accuracy. To prove its applicability for Direct Numerical Simulations, and therefore its ability to resolve the broadband scales present in turbulent systems, the DAWC method is used to study turbulent mixing in a simple turbulent flow, compressible decaying turbulence. Random blobs of two pure fluids of different densities areallowed to mix and the characteristics are analyzed. Of particular interest is the rate at which the heavy and light pure fluids mix, which has applications to the mixing on the two sides of the Rayleigh-Taylor mixing layer.

Norique Robles
University of Miami
HPC-2
Mentor: Douglas Hefele

Presentation Title: Mechanical Aspects Associated with Data Systems

Presentation Abstract: Supercomputers are at the forefront of complex and integral issues which LANL scientists and engineers deal with day in and day out. Since 1952 supercomputing machines have found their home at LANL; with the latest, codenamed Roadrunner, reaching speeds of approximately 76 trillion operations per second. The Strategic Computing Complex (SCC), a 300,000 sq-ft facility, has housed the newest generations of supercomputers and in May of 2008 will contain the world's most powerful supercomputer. However, most people do not understand the facility infrastructure of a computer room such as space, cooling, and electrical power. For continuous on-line usage, it is imperative to eliminate the immense amount of heat generated by the SCC's acre large computer room. The path of heat flow is traced to delve into the mechanical aspects in this computing facility. These aspects include heat transfer, systems and equipment, processes, and psychrometrics. Heat is generated within the computer then transferred to the air that enters an air handling unit, chiller, and finally exits out a cooling tower. Conduction and convection are the main types of heat transfer modes occurring. Systems and equipment allow for the heat transfer to occur and these include items such as heat exchangers, pumps, and fans. Processes such as evaporation, condensation, and the refrigeration cycles are the phenomena within the systems. Psychrometrics uses thermodynamic properties to analyze the conditions of air as heat is added and loss. By understanding the collective use mechanical aspects, one might begin to comprehend the magnitude of supporting supercomputers.

José Luis Rosales
New Mexico State University
PM-DO
Mentor: Gerard A. Montoya

Presentation Title: Remote Handling Waste Processing System

Presentation Abstract: The Atomic Energy Commission stated in a directive issued in 1970 that Transuranic (TRU) waste generated after 1970 must be stored in retrievable configuration until a deep geologic repository was available for its disposal. The Waste Isolation Pilot Plant (WIPP) opened on March 26, 1999 accommodates this objective. Los Alamos National Laboratory's post 1970 TRU waste is stored in shafts at TA-54 where the Decontamination/TRU Waste Support Team provides small item decontamination services, sorting, segregation, and recycling. This waste will be retrieved, characterized, and packaged for shipment to WIPP by 2012 as mandated. In conjunction with TA-54, CMR Waste Operations Team provides waste management guidance, visual examinations, and packaging of waste streams. To achieve the goal of packaging/characterization of TRU waste before sending it to WIPP, the team at TA-54 and CMR specified a process and guidelines to complete the task. To materialized the process and ensure deliverables the Applied Engineering and Technology (AET) team was assembled. The team's engineering capabilities are used to design and engineer the hardware for handling and processing transuranic waste. The handling process consists of a five stage system which uses alpha boxes in series to isolate waste remotely. During the first stage, a cask is used to transport waste to the processing area at CMR. The second stage consists of cutting the shaft in order to extract the contaminated waste. The third stage will analyze the waste and prepare it for separation. The fourth stage processes the waste and characterizes the gamma count. The final stage classifies the waste and packages it in drums in preparation for shipment to WIPP.

Zachary Shoemaker
Bradley University
D-3
Mentor: Michele DeCroix

Presentation Title: Design of a System to Manage Engine Exhaust Gas

Presentation Abstract: In the 2006-2007 school year, a senior project team was given a task to develop a system to manage engine exhaust gas from a 6.5-L, naturally-aspirated diesel engine. The project constraints are as follows: the exhaust must be projected in front of a Humvee-like vehicle at a maximum distance while having the capability to activate a passive infrared (PIR) sensor, and the exhaust system's effect on the engine's performance must be held below a 10% loss in power. Testing was performed on a diesel engine using orifice plates of varying diameters to restrict the exhaust and simulate engine back pressure. A pressure transducer and power-take-off (PTO) dynamometer were used to quantify the percent loss of power for each orifice diameter. The team used a thermal imaging camera to locate the thermal signature of the exhaust. It was found that an additional aerosol must be introduced to increase the distance from the vehicle to activate the PIR sensor. Los Alamos National Laboratory (LANL) and Bradley University have had a research relationship since August 2005. Each year LANL has sponsored senior projects in the mechanical engineering department. This relationship continues to produce quality research for the laboratory.

Brian Triplett
University of Florida
X-1
Kristen Triplett
University of Florida
HPC-1
Mentors: Morgan White & Doug Coomb

Presentation Title: Development of a Test Suite for Verification and Validation of Nuclear Data

Presentation Abstract: Verification and validation of nuclear data is critical to the accuracy of both stochastic and deterministic particle transport codes. In order to effectively test a set of nuclear data, the data must be applied to a wide variety of transport problems. The nuclear data team at Los Alamos National Laboratory (LANL) is developing a methodology to automate the process of nuclear data verification and validation. The International Criticality Safety Benchmark Experiment Project (ICSBEP) provides a set of criticality problems that may be used to evaluate nuclear data. The automation process applies cases from the ICSBEP benchmark set for testing of the developed methodology. This process is driven by an integrated set of Python scripts. Material and geometry data may be read from a Monte Carlo N-Particle (MCNP) input file to generate a standardized template or the template may be generated directly by the user. The user specifies the desired precision and other vital problem parameters. The Python scripts generate input decks for multiple transport codes from these templates, run and monitor individual jobs, and parse the relevant output. This output can then be used to generate reports directly or can be stored into a database for later analysis. This methodology eases the burden on the user by reducing the amount of time and effort required for obtaining and compiling calculation results.

Lucas Valdez
University of New Mexico
MQ-2
Mentor: Josh Montano

Presentation Title: Routine Performance Check for Optical Comparator Measuring Systems

Presentation Abstract: Optical comparators are calibrated, motorized machines that use light and magnification lenses to make non-contact dimensional measurements. Los Alamos National Laboratory's (LANL) Dimensional Inspection Team currently uses optical comparators in support of all major programs including Pit Manufacturing, Joint Test Assemblies (JTA), Life Extension, Surveillance, and Hydrodynamics. Current calibration cycles for optical comparators are two years. This is an optimal span based on cost of calibration, machine down time and machine history. Before calibration will recertify a machine, they perform an "as found condition" to verify the machine is still within its stated accuracy. If this check fails, and without a routine performance check, the data during the past two years would all be in question. The goal of the Routine Performance Check is to capture all the incidental things that may happen during a two year span. This includes but is not limited to bumping the machine, HVAC outages or temperature excursions, machine wear, drift, and lack of maintenance. The solution to minimizing the risk to product quality was a three prong approach. First, a calibrated inspection artifact was purchased. Second, a program was generated that could be run routinely with little effort. Third, data was output into a format for inspection personnel to monitor for changes. The result of this project has been viewed as both a cost savings and a success. Although it is hard to quantify actual dollars saved, the effort to run a routine check is significantly less than recalling or notifying two years worth of customers that their data is questionable. This has also allowed the inspection team to become more proactive in maintaining their equipment. Future work is to implement this program on all optical comparators and gather more data to produce more accurate run charts.

Mario Valdez
University of New Mexico
MQ-2
Mentor: Reina Ledoux

Presentation Title: Coordinate Measuring Machine - Machine Checking Gage

Presentation Abstract: Coordinate measuring machines (CMMs) are 3-axis machines that use a touch probe to measure points on a workpiece. CMMs are widely used throughout industry to ensure a workpiece meets drawing specifications. Los Alamos National Laboratory's (LANL) Dimensional Inspection Team currently uses CMMs in support of all major programs including Pit Manufacturing, Joint Test Assemblies (JTA), Life Extension, Surveillance, and Hydrodynamics. The current calibration cycle for CMMs is one year. This is an optimal span based on cost of calibration, machine down time and machine history. Before a machine is recertified a series of performance tests are conducted to verify if the CMM is still within the stated accuracy. If a CMM fails these performance tests the data taken during the past year is now in question. The goal of this work is to establish an interim check of the CMMs to capture all the incidental things that may happen during the calibration cycle. This includes but is not limited to bumping the machine, HVAC outages or temperature excursions, machine wear, drift, and lack of maintenance. The gage that was chosen to perform these checks is the Renishaw Machine Checking Gage (MCG). The gage is a commercial, off-the-shelf product developed to compliment existing standards for CMM volumetric performance testing. Data was collected daily on two Brown and Sharpe CMMs located at TA-3 and process control charts were developed. This gage has proven to meet the goal of this work.

MATERIALS SCIENCE

Andrea M. Dangelewicz
Clemson University
MPA-STC
Mentor:Yuntian T. Zhu

Presentation Title: "Annealing Hardening of Nanostructured Metals"

Presentation Abstract: Annealing of traditionally processed metals leads to softening, but it has been found that annealing of several nanostructured metals leads to hardening. Nanostructured samples of brass, pure aluminum, and pure nickel were prepared by severe plastic deformation. Differential scanning calorimetry was used to determine the recrystallization temperature of each material. Samples were then annealed below the determined temperature for different times and microhardness tested. Tensile testing and transmission electron microscopy will be used to explore the relationship between the resulting microstructures and hardness, strength and ductility. Several proposed mechanisms for annealing hardening include recovery of low angle grain boundaries, annealing twin formation, and reduction of dislocation density within grains.

Stephanie Sitarz
New Mexico Institute of Mining and Technology
MST-8
Mentor: Luiz Jacobsohn

Presentation Title: Synthesis and Characterization of Nanophosphors S.C. SITARZ, L.G. ACOBSOHN, B.L. Bennett, O. Ugurlu, R.E. Muenchausen, J.F. Smith, and D.W. Cooke

Presentation Abstract: Nanophosphors are nanosized, insulating, inorganic materials that emit light under particle and electromagnetic excitation. Their investigation revealed unique physical phenomena and great potential for technological applications. In particular, they can be used as scintillators for radiation detection in the Threat Reduction arena. Nanophosphors were prepared by solution combustion synthesis (SCS), taking advantage of exothermic redox reactions. Mixtures of metal nitrates and fuel undergo spontaneous self-sustaining combustion under heating. The chemical energy from the exothermic reaction heats the precursor mixture to high temperatures, forming a foam. The resulting material consists of macroscopic particles comprised of many nanocrystals fused to each other. Nanophosphors prepared using SCS by our team include: Y_2SiO_5:Ce, Gd_2SiO_5:Ce, Lu_2SiO_5:Ce,Y_2O_3:Tb, Gd_2O_3:Eu, and $Y_3Al_5O_{12}$:Ce. The goal of this work is to synthesize bright, high-quality powders of nanophosphors, consolidate them into bulk materials and study the structural, optical, and magnetic resonance properties. Several examples will be given to illustrate the importance of how changes in the SCS process parameters affect the nanophosphor structural and optical properties.

MATHEMATICS

Timothy Stone
Harding University
RP-1
Mentor: Michelle Lee

Presentation Title: Simulation of Airborne Contamination: Interpolation of Fixed Head Air Sample Data.

Presentation Abstract: At Los Alamos National Laboratory the air monitoring program is an integral part of the Radiation Protection Program which assists in worker safety at the Plutonium Facility. One primary method for evaluating airborne radioactivity is the use of Fixed Head Air Sampler (FHASs). The primary functions of FHASs are to verify integrity of engineering controls (i.e. gloveboxes and facility ventilation) and to provide a quantitative retrospective measurement of airborne radioactivity in the room. The FHAS are strategically positioned within the breathing zone of the worker at every other glovebox workstation; monitoring the containment of nuclear material with a high degree of sensitivity. The FHAS filters are replaced routinely and processed for airborne radioactivity. The purpose of this work is to provide a means of visual interpretation of the spatial FHAS data. These spatial data are interpolated and can be used to create a model illustrating the dispersion of contamination for a given room. The two favored methods of interpolation for these spatial data are the Radial Basis Function Multiquardic method and Kriging with a linear variogram. Many parameters can be modified within these methods making them both very robust in their applications. These methods are automated using Surfer® 8, a surface mapping program. The interpolation of the FHAS data will provide a statistically justifiable model for the dispersion of airborne radioactive contaminants. These models will be used to help interpret the FHAS data in the event of a release of airborne radioactivity.

Longhua Zhao
University of North Carolina at Chapel Hill
T-7
Mentor: Avadh Saxena

Presentation Title: Model of Air-Driven Mucus Clearance Mechanisms in Lungs

Presentation Abstract: Air flow through lungs may involve the presence of mucus which has much higher viscosity than air. To this end, we developed a model and examined the stability of two superimposed fluids with different viscosity in the two layers. Simple solutions of two-layer fluid flows with a high viscosity contrast can be unstable. This instability can be quite different than that occurring with a single fluid and in fact can shed some light on it when a perturbation approach is adopted. Our focus is on the limit of large viscosity contrast, which has not been fully analyzed or understood yet. Here the asymptotic properties of stability will be investigated. These results have a direct application in understanding air-driven mucus clearance mechanisms and the mucus transport phenomena in human lungs.

NON-TECHNICAL

Heather Altherr
The Evergreen State College
SEC-SIS2
Mentor: Luce Salas

Presentation Title: Environment-Safety-Security Poster

Presentation Abstract: Communicating security policies and procedures at the Laboratory is critical for increasing awareness about security requirements among employees. My work this summer involved helping in the development of the Annual Security Refresher by working with subject matter experts in Security Integration as well as Training. My other tasks included designing this poster, distributed Labwide and at the Nevada Test Site, which integrates environment, safety and security messages. In our modern society images are increasingly used to raise awareness of specific topics. However because people are so overwhelmed with visual stimuli it has become harder to attract and focus the crowds attention. In my case I wanted to send a message concerning environmental, safety, and security issues in an eye-catching and sophisticated way. I have achieved this by giving the poster a futuristic look using bright colors and curved smooth shapes. I used a Photoshop as well as InDesign to create the result.

Jennifer Purdy
University of New Mexico, Los Alamos
CTN-4
Mentor: Denise Lopez

Presentation Title: Description of Mission Statement, Objectives and Strategic Planning for CTN-4

Presentation Abstract: CTN Telecommunications Group designs, develops and installs the labs telecommunications. The purpose of my poster is to discuss CTN-4's mission, our goals and our achievements. During my presentation I will explain some of the key things telecommunications does and how it relates to CTN-4's mission and objectives as well as the lab's mission and objectives.

Bethany Rendell
American Military University
SEC-SIS2
Mentor: Charles Campbell

Presentation Title: The Defense Nuclear Security Lessons Learned Center

Presentation Abstract: The National Nuclear Security Administration (NNSA), Office of the Associate Administrator for Defense Nuclear Security (NA-70), established a centralized Defense Nuclear Security Lessons Learned Center (DNS-LLC) at Los Alamos National Laboratory (LANL). A primary goal of the Associate Administrator for DNS is to ensure that experiential information is shared among NNSA sites to promote innovative approaches to encourage outstanding security practices and to avoid the recurrence of adverse security practices. The purpose of a lessons learned program is to share and use knowledge for continuous improvement by avoiding recurrent or similar problems and encouraging and reinforcing secure practices. Lessons learned should be available at the worker and supervisor level to be an effective tool in preventing recurring problems and supporting secure work practices.

PHYSICS

Brent Apgar
University of Washington
Inst-Off-MDI
Mentor: Don Brown

Presentation Title: Deformation modes and activities and texture analysis of stoichiometric β' AuZn using in-situ and ex-situ neutron diffraction

Presentation Abstract: Shape-memory alloys (SMA) are finding increased application in fields as diverse as transportation, medical treatment, and consumer products. Despite this broad usage, the fundamental thermodynamics of the shape-memory effect and the cause of SMA behavior have yet been completely explained in detail. Stoichiometric β' AuZn is a shape memory alloy that transforms from its austenitic B2 cubic phase to martensitic P3 trigonal phase at 64.8K. In-situ and ex-situ measurements of lattice strain and texture during plastic deformation in compression were made using neutron diffraction in the Spectrometer for Materials at Temperature and Stress (SMARTS) and the High Pressure Preferred Orientation (HIPPO) instruments at the Los Alamos Neutron Science Center, Lujan Center. Samples were prepared by swaging at 300° C, followed by annealing at 250° C for 1 hour, and machining to produce cylinders approximately 0.4 cm3. Measurements were made prior to and after deformation in HIPPO and during deformation in SMARTS. The lattice strain and grain texture were calculated by single peak fits and Rietveld refinement of the diffraction patterns. The fitted diffraction patterns allowed the texture from processing, deformation modes and activity, and texture development during deformation to be determined. AuZn experiences a local maximum in ductility at room temperature, therefore, samples were deformed at high and low ductility points, 25° and 100° C respectively, to compare the deformation modes and activities and determine the cause of the variation in ductility.

Maria Castro
University of Illinois at Chicago
P-25
Mentor: Gerd J. Kunde

Presentation Title: CMS Detector Effects on the Measured Z0 Mass Distribution

Presentation Abstract: There is strong indication that a new state of matter, the Quark Gluon Plasma (QGP), is created in relativistic heavy ion collisions. The analysis of hadron jets via leading hadron correlations has been an effective probe into the properties the QGP medium. Jet analysis has allowed the study of back-to-back partons that fragment into hadron jets. Up until now, the energy of the initial parton scattering remains unknown because the hadrons strongly couple to the medium and lose energy before they can be measured. At LHC energies, the rates for parton-parton interactions that produce Z0 bosons with subsequent decay into lepton pairs and associated hadron jets make the study of Z0-tagged jets possible. Since the leptons are electromagnetically interacting, they do not lose energy traversing the medium, i.e. they don't couple to the strongly interacting medium. Their measured kinematics gives direct access into the initial energy of the opposite side hadron jet and thus offers, for the first time ever, direct measurement of in-medium effects. The experimental signature is provided by the measurement of muon pairs from Z0 decays, for which CMS is an ideally suited detector. In this study, the affects of several CMS detector effects on the Z0 mass distribution are shown.

Andrew Grieco
New Mexico Insitute of Mining and Technology
DE-9
Mentor: David Moore

Presentation Title: Precision Raman Spectral Analysis of Pre-1300 A.D. Redware Pottery Shards

Presentation Abstract: Redware pottery shards from the three major pre-1300 A.D. traditions were analyzed using a DeltaNu InspectorRaman portable Raman spectrometer. Spectra were acquired over extremely long exposure times to improve precision, and features resulting from mineral vibrational modes were isolated using ambient light subtraction followed by a rolling-circle filter to eliminate the remaining background signal. For each tradition the nature of the pigmentation (organic or inorganic) and the type of firing atmosphere (oxidizing or reducing) were determined.

Samuel Harrold
University of Rochester
P-24
Mentor: Glen Wurden

Presentation Title: Multi-element Magnetic "B-dot" Probe

Presentation Abstract: We describe a 30-element magnetic probe consisting of miniature commercial chip inductors that will be used to investigate the evolution of the magnetic field lines during a reconnection event. Ten clusters of three mutually orthogonal inductor coils mounted in a linear array provide dB/dt data in the x, y, and z directions with a spatial resolution of 0.5 cm. The probe will be part of the Reconnection Scaling Experiment (RSX) at Los Alamos National Laboratory, which creates multiple magnetic flux ropes of H plasma. Using a numerical integrating circuit, we expect to measure magnetic field strengths of 1-10 gauss with a probe sampling rate of 20 MHz. The plasma columns of RSX that undergo magnetic reconnection evolve on a characteristic timescale of 1-10 μs, well within the probe's expected time resolution.

Robert Haussman
Massachusetts Institute of Technology
P-21
Mentor: John Chiaverini

Presentation Title: Ion-trap potential calculation for large-scale quantum information processing

Presentation Abstract: The trapping and manipulation of individual atomic ions has important applications in quantum information processing (QIP). In particular, quantum simulators, which directly emulate inaccessible quantum systems that are intractable to simulate classically, may be some of the first practical devices to exploit QIP. Radio frequency (RF) Paul traps that make use of an oscillating quadrupole field created by a four-rod architecture are typically employed for trapped-ion QIP. Surface electrode traps offer significant advantages over this type of trap due to their compatibility with microfabrication and ease of integration with control electronics. However, these traps suffer from low trap depths and reduction of trapping frequency, necessitating numerical optimization in the design. To aid in construction of large-scale trap arrays, we explore two techniques that offer significant improvements in calculational efficiency and accuracy compared to traditional techniques such as relaxation and finite element techniques. First we apply the boundary element method (BEM), which partitions the electrode into a mesh of charges from which the electric field is then easily calculated via Coloumb's law. Next we apply a technique that maps the traditional Dirichlet problem onto a simpler Biot-Savart-like problem in which we consider a hypothetical current loop traced out by the electrode boundary. This method often allows for analytical results to non-trivial electrode configurations. Both methods are compared to each other and to theoretical and experimental results previously obtained. These calculations are then utilized to design multizone traps for 1-D (and possibly 2-D) quantum spin system simulations.

Jennifer Hendryx
Angelo State University
P-24
Mentor: Glen Wurden

Presentation Title: Calibration and Alignment of High Resolution Spectrometer for use on FRXL and RSX Plasma Experiments

Presentation Abstract: Measurements of ion temperature and plasma flow are important for better understanding of laboratory plasmas. Plasmas are the key to production of nuclear fusion, and plasma diagnostics are essential for experimental plasma studies. Spectroscopy in particular is useful in analyzing plasma temperature, flow, and impurity content. It utilizes spectral lines' widths, intensities, and locations in the spectrum to determine elements present in the plasma, as well as line shifting and broadening that occur, for example, due to ion thermal motion—Doppler broadening. I assembled and calibrated a 0.5 meter McPherson VM505 spectrometer, combined with a 1024x1024 element gated intensified PI-Max camera as a detector, to view plasma light from the RSX and FRX-L experiments in the P-24 Plasma Physics group. With a 1200 line/mm grating, the resolution FWHM is 0.03 nm, and initial data looking at the 486.1 nm deuterium beta line will be presented.

Mark Herrera
University of Missouri, Rolla
T-CNLS
Mentor: David Roberts

Presentation Title: Complex Networks and Scientific Ideas: The Road to Revolution

Presentation Abstract: From time to time, scientific revolutions take place which connect different disciplines to form new, independent subfields. For example, papers in the 1980s connected the distinct fields of information theory and quantum mechanics into quantum information theory. A question naturally arises when studying the merger and creation of new scientific revolutions: is there any way to develop a quantitative understanding of this evolving network of scientific ideas? In recent years, new understandings of many complex systems in physics, biology and even the social sciences have been gained through the application of network theory. Once can build a network of ideas from a scientific paper database, where nodes are subject classifications assigned by that database, and links are formed when two subjects appear in the same paper. By applying the developed tools of network theory, such as edge prediction and community detection to these idea networks, this study aims to address the question of whether or not it is possible to predict the creation of new subfields.

William Kindel
University of Colorado, Boulder
X-1-PTA
Mentor: Christopher Rousculp

Presentation Title: Axial Radiation Optimization on Sandia Z-Machine Using 1-D Computations

Presentation Abstract: The axial radiation emitted during Z-pinches on Sandia Zmachine is optimized using RAVEN, a 1-D magnetohydrodynamic (MHD) code, by varying wire array parameters. Z-machine's axial radiation is used for inertial confinement fusion experiments. The Z-pinches are modeled with RAVEN by solving a lumped-element circuit model driven with a time-dependent voltage pulse coupled with an azimuthally symmetric, cylindrical shell of plasma, which represents the wire array. In the optimization, the plasma shell's mass at constant length, the radius, and the material composition (Al, Cu, Ag, and Stainless Steel) are varied. The results of the optimization will be shown.

Michael Krantz
Rose-Hulman Institute of Technology
MST INST-OFF
Mentor: Steve Valone

Presentation Title: A Theoretical Study of the elastic Properties of AuZn

Presentation Abstract: AuZn is a thermoelastic martensite which exhibits several interesting characteristics. A few of these qualities include a very low phase transition temperature of 64.8K and the appearance of a second-order transition in stoichiometric AuZn. These anomalies have provoked a growing interest in the material. As a result it was selected as the topic of study for the Material Design Institute summer school program. Our interest is in looking at the physical properties, particularly the elastic constants, of AuZn from a theoretical perspective. In order to do this we will use the Vienna Ab-initio Simulation Package (VASP), an electronic structure computational program, to perform energy calculations for specified strains. Initially we will consider an ideal stoichiometric system. Then we will look at the effects of point defects and nonstoichiometry on the physical properties of the material.

Christopher Leibs
Rose-Hulman Institute of Technology
P-24
Mentor: Glen Wurden

Presentation Title: An Investigation of Mach-Zehnder Interferometry as a Diagnostic for Field Reversed Configuration Plasmas

Presentation Abstract: The Field Reversed Experiment-Liner (FRX-L) produces Field Reversed Configuration plasmas (FRCs) that will be translated into a liner implosion system where they are compressed to thermonuclear conditions. Being able to accurately determine the translational velocity as well as the electron density of the FRC prior to its introduction to the implosion system is crucial. With life times on the order of 10 microseconds, densities ranging from an order of 10^15 - 10^17 / m^3, and large amounts of magnetic, electrical and acoustic noise, measurement systems have to be fast and robust. Two types of interferometers are being investigated for their ability to quickly and accurately measure these plasma properties during the translation period. Both are single pass Mach-Zehnder interferometers. The first is a quadrature interferometer employing a linearly polarized scene beam coupled with a circularly polarized reference beam. The signals produced will be proportional to the sine and cosine of the phase shift introduced by the plasma. This interferometer will operate at 1330 nm and will work within fiber optic cables. The second will be an air-path 633 nm He-Ne interferometer. It will exploit the properties of an acousto-optic modulator (AOM) to split the beam, as well as produce the desired frequency shift in the scene beam. When recombined the time-varying sinusoidal signal can be demodulated to produce, again, the sine and cosine of the phase delay produced by the plasma. While both interferometers are used to accomplish the same task, each has its advantages and disadvantages.

Niall Mangan
Clarkson University
T-CNLS
Mentor: Cynthia Reichardt

Presentation Title: Intermittency in Nonlinear Dynamics: AC Driven Vortices

Presentation Abstract: Using numerical simulations, we study superconducting vortices shaken by an ac drive in the presence of a random pinning substrate. Even in the absence of thermal fluctuations, we observe both reversible and irreversible regimes of vortex motion. Intermittent transitions between the two regimes occur at a frequency which is determined by the vortex density as well as the amplitude and period of the driving force. We also observe a smectic flow regime in which vortices diffuse along the direction of the drive but undergo reversible behavior perpendicular to the drive.

Sara Martin
University of New Mexico
P-21
Mentor: Michelle Espy

Presentation Title: A Magnetophoresis Instrument for Sorting Magnetic Microparticles

Presentation Abstract: Our goal is to demonstrate a highly parallel, sensitive technique for quantitative molecular analysis that will expand current biomedical research capabilities. A magnetophoresis instrument was built and characterized using a flow chamber in a magnetic field gradient to sort magnetic microparticles. The microparticles will eventually be used as biological labels. The flow chamber consists of a sample inlet, differential sheath streams, and eight outlets for collecting the microparticles after they have traversed the chamber. Magnetic microparticles are injected into the flow chamber that is positioned in a linear magnetic field gradient. The trajectory for each microparticle is determined by magnetic moment and diameter, resulting in populations of microparticles that have been sorted according to magnetic moment. The system has been characterized for sorting superparamagnetic and ferromagnetic microparticles with diameters of 8 µm and 4.0 – 4.9 µm, respectively, by varying their transit time through the chamber. The ability to reproducibly change the distribution of the particles in the collection bins by this method was demonstrated in good agreement with theory. Design improvements, such as reducing the aspect ratio between sample inlet and chamber depth and stabilizing the sheath flow, resulted in narrow sorting distributions. For the eight outlet chamber, a sorting reproducibility (particles returning to the same bin upon resorting) was measured to be 84-89%. We are currently investigating flow chamber designs that will allow sorting magnetic microparticles into as many as twenty-five outlets, while maintaining hydrodynamic stability.

Roy Murray
New Mexico Institute of Mining and Technology
PMT-3
Mentor: James Pecos

Presentation Title: Gamma Ray Detection

Presentation Abstract: The detection of gamma radiation plays an important role in personnel safety and security at Los Alamos National Laboratory as well as in the protection of the environment. A new gamma ray detector was released fairly recently. The one that is in use currently has been the top of the line for the last 20 years, but the new one seemed to be a possible competitor. A study needed to be done to compare the two and determine which to purchase and use. To accomplish this task the two detectors were used to measure the same source of gamma radiation. The source chosen was a small piece of plutonium foil, which produces a wide energy range of gamma rays. The detectors were compared in three categories: efficiency, resolution, and energy calibration. Efficiency is a measurement of how many incoming gamma ray photons are picked up by the detector, which can be directly compared. Resolution is a measurement of the width of an energy peak at half of its maximum value, also directly compared. Energy calibration involves plotting energy peaks in Microsoft Excel and comparing the linearity of the curves. The HPGe detector performed better in all categories, with performance up to 67 times better than CZT. With this information, the HPGe detector will continue to be used for measurements inside of the Plutonium Facility.

Levi Neukirch
University of Nebraska
P-25
Mentor: Dale Tupa

Presentation Title: An exploration of Rb optical pumping properties at low buffer gas pressures

Presentation Abstract: The optical pumping of alkali metals has been studied for high buffer gas pressure regimes. The resulting polarized vapors are useful in a number of fields including medical research and basic science. Typically, a buffer gas such as N2 or He is mixed in with the alkali vapor to quench radiative decay processes and limit radiation trapping, limit the diffusion of the metal atoms to the depolarizing pumping cell walls, and provide the benefit of homogeneously broadening the absorption spectrum of the metal. Homogeneous broadening allows effective pumping of a broad absorption spectrum with a laser whose spectrum is too narrow or composed of discrete frequency modes. For these purposes, buffer gas pressures range from hundreds of torr to several atmospheres. Such pressures, while advantageous for the optical pumping process, can be detrimental for certain experiments. For instance, in an electron spin filter device where an electron beam must traverse the pumping cell, buffer gas pressures in excess of a few torr severely reduce beam currents. Our group is currently working on such a device using rubidium as our optically pumped alkali metal. Previous studies have shown N2 to be an effective buffer gas in the pressure range of 0.1 to 50 torr. Using sealed glass cells with varying pressures of nitrogen we conducted studies of rubidium polarization versus rubidium number density and pump intensity. An overview of optical pumping is presented along with a summary of our results and measurement processes.

John Ogren
University of New Mexico
P-23
Mentor: Justin Torgerson

Presentation Title: Frequency Quadrupled Laser System for Ytterbium 2+ Spectroscopy

Presentation Abstract: In the case presented, Ytterbium2+ (Yb2+) was being sought in a linear RF trap. In order to detect and then laser cool the Ytterbium2+, the 1S0 to 3P1 (???) transition at 252 nm was chosen due to the fast transition period of 231 ns. In order to excite this transition a laser system at 252 nm was needed that was widely tunable and had a narrow linewidth. There were no commercially produced laser systems that fulfill these requirements. The proposed solution to this problem was to frequency quadruple a commercially available Titanium-Sapphire (Ti-Sapph) laser from 1008 nm to 252 nm. The titanium doped sapphire crystal was within a monolithic block resonator (MBR) and, when lasing, was tunable over a wide range of wavelengths (approximately 700 nm to 1100 nm) with a linewidth of approximately 100 kHz. This provided the necessary flexibility needed for the spectroscopic and cooling applications. A Potassium Niobate (KNbO3) crystal was mounted within the MBR cavity and frequency doubled the initial Ti-Sapph beam from 1008 nm to 504 nm. The resulting beam was then doubled again using an external doubling cavity with a β-Barium Borate crystal (BBO). Currently, 12 W from a Diode Pumped Solid-State Continuous Wave (DPSS CW) laser, operating at 532 nm, pumps the MBR which produces roughly 50 mW at 503 nm through the KNbO3. As of recently, 2 mW of power has been output from the BBO. In addition, the linewidth is no more than 400 kHz and is tunable over several GHz. These excellent results encourage the use of frequency quadrupling techniques to retain the original characteristics of commercial lasers while fitting the system to the specific needs and goals of a project.

Daniel Olive
Illinois Institute of Technology
EES-12
Mentor: Donald Reed

Presentation Title: Analysis of Environmentally Relevant Solids/Phases using Synchrotron-Based Methods

Presentation Abstract: Synchrotron-based methods were used to establish the oxidation state and, in some cases, the phase, of environmentally relevant actinide and lanthanide precipitates and phases. This is a key focus of the EES12 Actinide Chemistry Repository Science Program (ACRSP) research at the Carlsbad Environmental Monitoring and Research Center (CEMRC). This work supports ongoing recertification of the Waste Isolation Pilot Plant (WIPP), the only working US nuclear waste repository, and general actinide migration issues at DOE sites. Plutonium, uranium, and neodymium, as an analog for Pu^{3+} and Am^{3+}, samples were investigated. Samples were encapsulated in Kapton film, and maintained in an inert Ar atmosphere. Analyses were performed at Argonne National Laboratory's Advanced Photon Source (APS) MR-CAT beamline; which employs an undulator fed Si(111) monochrometer, and uses a combination of ion chambers and solid state detectors to measure absorbance in both the transmission and fluorescence modes. There was no uncertainty about the oxidation state of neodymium in our WIPP Brine experiments. Emphasis was on EXAFS to establish the structure, to the extent possible, of the actual precipitates that were observed in the long-term solubility studies performed. For uranium and plutonium, the key issue was the redox distribution of the actinide as a consequence of the microbiological and Fe interactions observed in the reduction experiments – so the main emphasis was on XANES edge analysis to establish the oxidation state distribution. In our experiments, U(VI) and Pu(V/VI) were reduced to U(IV) and Pu(III/IV) respectively showing that lower oxidation states of these multivalent actinide will prevail under iron rich or microbially active anoxic conditions.

Ian Percel
University of Illinois, Urbana
Jennifer Webster
University of California, San Diego
X-3
Mentor: Richard Nebel

Presentation Title: S7 Variance Reduction for Radiation Transport

Presentation Abstract: Radiation hydrodynamics is employed by physicists to describe the behavior of fluids that are strongly coupled to a radiation field. This is particularly important in analyzing astrophysical phenomena. Direct Simulation Monte Carlo is one of the few numerical tools available for solving realistic problems in radiation hydrodynamics. Since M. Kotschenreuther's work in 1988, the δf method has dramatically reduced the variance observed in Monte Carlo solutions to problems in plasma physics. Recently, researchers at Lawrence Livermore National Laboratory (LLNL) have considered using a similar technique in radiation transport. The new algorithm being studied at Los Alamos National Laboratory (LANL) includes the LLNL algorithm as a special case. The LANL equilibrium term results from using the standard asymptotic expansion to include diffusion as well as the Local Thermal Equilibrium component that the LLNL algorithm is restricted to. The weighting function is evolved using a difference equation for the total time derivative of the distribution. The connection to the weighting function is established by using a Klimontovich epresentation of the system. In this research, the proposed change has been formally proven to provide a valid extension of the δf method. The derivation also implies the existence of an alternate evaluation method that may provide a check on the diffusion approximation. If efficiency gains observed in plasma physics simulations hold, the new algorithm should show a dramatic improvement over the LLNL algorithm. Specifically, the new algorithm may offer as large a gain in efficiency over the LLNL algorithm as the LLNL algorithm demonstrates when compared with analog methods. A comparison of the two algorithms has not been completed and continuing work should provide a basis for further improvements. This algorithm may offer significantly more accurate radiation transport calculations than have been possible to date. Initial numerical results will be presented.

Leslie Sasa
University of California, Los Angeles
LANSCE / LANSCE-LC
Mentor: Rex Hjelm

Presentation Title: Neutron Reflectivity Studies of Polymer Response to Shear

Presentation Abstract: We have built a neutron stroboscopic rheometer (NSR) to study non-linear polymer dynamic response to stress. The NSR provides the ability to provide high torque (200 Nm) at shear rates of up to 100 Hz in a cone and plate configuration. Using neutron reflectometry and deuteration to discriminate substrate-bound polymer brushes from the bulk polymer melt, we have made the first measurements on the molecular basis of polymer slip-shear by providing a new physical description of polymer behavior at interfaces. Our objective is to test the notion of deGennes, which describes the coupling between the dynamic response of the bound brush and the bulk material. The density profiles of our first measurement of bound protonated poly(dimethylsiloxane) (PDMS) against deuterated bulk PDMS revealed two layers: a thin layer of protonated polymer at the surface of the substrate and an intermixed layer, where the brush is not only mixed in with the deuterated melt but most likely entangled with it. As shear was applied to the system, the entangled brush layer lengthened. At even higher shear rates, this intermixed layer began to shrink again, suggesting the start of disentanglement. Our results, while in agreement with the deGennes model, provide more detail on the events leading to slip-shear. In our next set of experiments, atom transfer radical polymerization (ATRP) will be used to produce uniform, thick polystyrene (PS) brushes. We have done some preliminary testing on these samples to test their swelling behavior. Preliminary tests indicate that better PS brushes are made using this technique.

David Sirajuddin
University of Michigan
P-24
Mentor: Scott Hsu

Presentation Title: Generation and Measurement of Magnetic Fields for the Driven Relaxation Experiment

Presentation Abstract: The Driven Relaxation Experiment (DRX) aims to study driven magnetic relaxation in plasmas, i.e., the evolution of a magnetized plasma toward a nearly "force-free" sustained state where currents and magnetic fields are nearly parallel. This poster will describe the motivation, design details, and assembly process of three hardware systems: (1) a "flux loop" which will be used to calibrate the "bias" magnetic flux generated by an external coil set; (2) a pulsed capacitor bank power system to drive current in the external coil set; and (3) small magnetic pickup loops to measure the magnetic field on the plasma boundary, which will help us infer information about the existence and evolution of internal plasma modes. Time permitting, we will obtain and show experimental data from these systems.

Joshua Spencer
University of Illinois
X-1 HEDPL
Mentor: Greg Pollack

Presentation Title: Parallelization of a Post-Processing Code for Cutting-Edge Rad-Hydro Codes Using MPI

Presentation Abstract: Today one of the most active areas of research in high performance computation is in computational fluid dynamics (CFD) and in particular radiation hydrodynamics. Radiation often plays a large role as an energy transport mechanism in the plasmas of interest to the community. This radiation can be used to diagnose the state of the plasma being studied, and can also be used for radio graphic purposes. The post-processing code being studied here, Plaspp, utilizes a ray-tracing approach to handle the radiation transport, as opposed to Monte Carlo photon transport and in doing so is considerably faster. In 3D Eulerian simulations, extremely large arrays occur, consistent with many x10^{8} zones. Therefore these are huge problems with vast amounts of data, so to efficiently post-process them requires parallelization of the problem over many different processors. For very large problems rad hydro codes when outputting their data, can use Ensight graphics dumps to decompose the run domain into smaller sections. The work presented here describes the process of setting up Plaspp to run these smaller domains in parallel using advanced MPI-2 spawning techniques.

Dustin Spieker University of Missouri, Rolla
DE-9: Detonation Physics
Mentor: Mark Short

Presentation Title: Numerical Modelling of Gas-Gun Experiments in SX 358 Foam Using AMRITA

Presentation Abstract: The response of foams to shock compression at high pressures and shock velocities (pressures on the order of GPa and shock velocities on the order of km/s) is not yet fully understood. The characterization of the shock response of materials in this class is important. The Hugoniot curve, the locus of all end states permissible by shock compression, is an important characteristic of the response of materials to shock compression. It can be experimentally determined using gas-gun experiments, in which a flyer plate of a known material is launched at high velocities towards a sample of the material of interest. One such material is SX 358, a PDMS based filled foam. The particle velocity in the sample material is then measured using embedded electromagnetic “stirrup” gauges. In recent experiments, large displacements of the particle velocities were observed in the SX 358 material. The aim of this project is to determine (i) the origin of the velocity displacements, and (ii) extract information on the frozen sound speed of SX 358. The difference in material properties between the gauge material and the test material, or the influence of air gaps between the gauges and material, are two possible causes bethind the velocity diaplacements. Using the adaptive mesh refinement code, AMRITA, the interaction between the projectile, the test material and the embedded gauges is modeled numerically. The difference between the velocity profiles with and without the embedded gauges can then easily be investigated. The physical response of the material must be modeled and so the numerical modelling also serves as a test of the validity of the SESAME table used as an EOS for SX 358.

Shawn Tomga
University of New Mexico
ISR-1
Mentor: John Sullivan

Presentation Title: Imaging Algorithms via List Mode Maximum Likelihood Expectation Maximization and the Prototype Compton Imager

Presentation Abstract: Compton imaging is a gamma ray imaging technique that has possible applications in the nuclear and medical industries. Compton imaging can localize the origin of a scattered gamma ray, to a cone, using a minimum of 2 position and energy measurements. The projection of many cones will overlap at a common point leading to the actual source position. This method applies to both point and extended sources. Current back-projection algorithms employed by the Prototype Compton Imager (PCI) are not sufficient to resolve extended shapes, however iterative algorithms may provide the necessary deconvolution. Maximum Likelihood Expectation Maximization (MLEM) is an iterative algorithm that reconstructs the most probable source distribution for a given data set. A drawback of the MLEM algorithm is the large amount of computation time required for image convergence. Because iterative algorithms make computations for each possible combination of energy and position this becomes a prohibitively large problem for both analysis time and memory limits. List Mode MLEM attempts to circumvent the calculation of every combination of energy and position and relies on the probability of the given data being observed. An algorithm using List-Mode MLEM is of interest because the number of calculations required for reconstruction is substantially less than that of other iterative processes but will enable imaging of extended source. This type of algorithm has been written and successfully applied to both experimental data from the PCI and simulations of the PCI. The algorithm has been used for both point sources and extended sources.

Carl Wilde
University of New Mexico
P-23
Mentor: Gary Grim

Presentation Title: Recent Results in ICF Neutron Imaging using a 9 pinhole array

Presentation Abstract: Neutron imaging (NI) provides a powerful diagnostic for understanding the performance of ICF ignition targets and the drive mechanism imploding them. To achieve the spatial resolution and signal-to-noise ratio required of the National Ignition Facility (NIF) requires a signal multiplexing imaging system. One such imaging approach is pinhole array imaging. In this paper we present results from analyses of neutron images formed with a 3×3 array of identical pinholes. The images were formed using directive implosions of deuterium and tritium filled CH targets with the Omega Laser at the University of Rochester, Rochester, NY. We describe the innovative techniques developed to manufacture the pinholes, the experimental conditions under which the images were taken, the algorithms used to perform the analyses, as well as a comparison with simulated image performance.

Thomas Wong
Santa Clara University
T-4
Mentor: Matt Foster

Presentation Title: Calculation of Elastic Differential Cross Sections for Proton-Helium Collisions Through the Use of High Performance Computing

Presentation Abstract: A solid theoretical framework for describing ion-atom collisions is crucial for understanding fusion environments. From basic atomic collision theory, the differential scattering cross section can be expressed in terms of the scattering amplitude, which can be expanded in partial waves. Existing computational efforts to calculate these cross sections are in disagreement with experimental results. Recently, however, accurate electron-atom collision results were produced by taking into account the electron screening of the atom. This project uses the high-performance computing resources available at Los Alamos National Laboratory calculate the elastic scattering cross sections for ion-atom collisions while taking into account electron screening. This is numerically challenging compared to electron-atom collisions, since neither the ion's nor atom's mass is negligible, whereas an electron's mass would be. Efforts to develop this project are still underway, and results are not yet available.

TECHNICAL TALKS ABSTRACTS

SYMPOSIUM 2007

BIOSCIENCE

Jordan Atlas
Cornell University
T-10
Mentor: James Faeder

Presentation Title: Comparison of a Rule-Based and a Traditional Pathway Model of a Signal Transduction System

Presentation Abstract: Cells make decisions based on the output of complex signaling pathways triggered by the presence or absence of some chemical signal in the environment. These decisions have anywhere from minor to drastic effects on cell behavior, and the response to different levels of chemical signal is highly non-linear. Signaling involves a myriad of protein-protein interactions which give rise to a combinatorial number of protein complexes and states, and explicitly modeling this large number of complexes is usually not possible. Consequently, modelers often make simplifying assumptions that greatly reduce the number of species in the network under study. Rule-based modeling is a method for generating a biochemical reaction network from an abstract description of the reactions in a biological system. Reaction rules define both the class of reaction associated with a particular type of interaction, and the kinetic rate-law for that reaction class. Using a rule-based modeling approach allows a modeler to explore the effect of including combinatorial complexity in a signal-transduction network, but it is still unclear what the fundamental differences between an analysis produced by rule-based and standard approaches are. In this study we compare two models of events in signaling caused by the epidermal growth factor (EGF) receptor (EGFR). In particular, we use the SloppyCell software environment to perform parameter distribution studies and compare how data constrains the feasible output spaces for the two models. The overall goal of this project is to examine the extent to which parameter estimates for rule-based models can be refined based on qualitative observations.

Joshua Hanson
University of California, Davis
MPA-CINT
Mentor: Andrew Dattlebaum

Presentation Title: Cell Endocytosis of Fluorescent Silica Nanoparticles

Presentation Abstract: Silica nanoparticles containing a variety of ruthenium polypyridyl dyes were imaged in biological systems using both wide-field and confocal microscopies. The silica nanoparticles studied here may eventually serve as biomarkers for intracellular tracking and sensing, or as vehicles for drug delivery. The nanoparticles ranged in size from 20 to 50 nm and contained fluorescent molecules that emitted in either the visible or the near infrared region. Differentiated human monocytic cells (THP1) were exposed to varying concentrations of the nanoparticles for 60 min, following which the cells were fixed and imaged to determine the level of uptake by the cells. Cross sectional measurements taken using confocal microscopy to image the endocytosis of the silica nanoparticles by macrophage-like cells will be described.

Paulina Zelenay
University of Texas, Austin
LANSCE-LC
Mentor Jaroslaw Majewski

Presentation Title: X-Ray Scattering Investigations of Siderophores Interacting with Model Biological Membranes

Presentation Abstract: Iron is essential for the growth, proliferation and pathogenicity of microorganisms such as bacteria. Competition for iron between a host and bacteria is one of the most important factors determining the course of a bacterial infection. The biosynthesis and secretion of siderophores is one common strategy many bacteria employ to obtain iron from their environment. In spite of the wealth of information on siderophores from diverse microbial species, detailed information on their entry into cells following binding of iron is not completely understood. The knowledge of this process may be employed to use siderophore entry as means to deliver other cargo, such as antibacterial compounds, into cells. In this study we made model membranes composed of different phospholipid monolayers (Langmuir layers) at the air-water interface and used pressure-area isotherms to measure changes in the lipid packing properties upon interaction with siderophores. In order to get high-resolution insight into the properties of the system we used synchrotron x-ray reflectivity and grazing incidence x-ray diffraction to monitor in-plane and out-of-plane changes in density distributions of the lipid membrane. Our investigations show that there are only small changes in membrane ordering during interaction with siderophores. This supports the claim that the presence of trans-membrane proteins is required in order to facilitate siderophore transfer through the cell membrane.

CHEMISTRY

Raea Hicks
University of Colorado, Boulder
MPA-CINT
Mentor: Andrew Dattelbaum

Presentation Title: Preparation and Luminescence Studies of Ru (II) Polypyridyl Complexes in Silica Nanoparticles.

Presentation Abstract: Human blood and tissue absorb light at wavelengths less than 700 nm and greater than 1,000 nm. There is need for bio-compatible tracers that absorb and emit light within the biologically transparent window between these wavelengths. To address this problem, we encapsulated near-infrared (NIR) emitting Ru (II) complexes into silica nanoparticles (diameter = 20 and 50 nm) using the inverse-micelle emulsion method. The nanoparticles were also coated with hydrophilic silanes for improved solubility and monodispersity in water. Visible and NIR fluorescence spectra of the complexes in solution and encapsulated in nanoparticles reveal a blue-shift in silicaencapsulated dyes, which is explained by the rigid-medium effect. Overall, we succeeded in making nanosized tracers with desired photochemical and biological properties**.**

COMPUTING

Colby Boyer, University of California, Berkeley
HPC-5/CTN-5
Mentors: Robert Martinez, HB Chen

Presentation Title: Comparison of 10GigE and InfiniBand Interconnects

Presentation Abstract: The goal of a high performance supercomputing cluster is to achieve the highest possible performance using generic parts to the lowest cost. InfiniBand is currently used to maintain low latency and high bandwidth though the recent 10GigE standard offers considerable improvement over its predecessor in both bandwidth and latency performance and might be a viable option. Our driving question is whether or not 10GigE will be price and performance competitive with InfiniBand. Our objective is do a comparison between two cluster interconnect cut through switches: InfiniBand and Fujitsu 10GigE. This will be done by benchmarking the latency performance, throughput performance, cost, and scalability using MPICH2 over InfiniBand over IP and MVAPICH2 over native InfiniBand. We hope our results will show whether 10GigE is a viable interconnect for high speed computing applications.

Matthew Brock
Texas State University
HPS-4
Mentor: David Montoya

Presentation Title: Tree-Based Overlay Networks in High-Performance Computing

Presentation Abstract: Scalability is a significant concern in the context of highperformance computing. One approach to achieving performance gains in HPC environments is the addition of physical resources (compute nodes, memory per node, etc.) The downside to this approach is that it is not necessarily a solution in and of itself. The software performing computations in this environment must leverage these additional resources in order to meet performance gain expectations. Communication between nodes is one of the many issues and complexities impacting software scalability. A common overlay network topology in node communication is a single node (referred to as a front-end) directly connected to many nodes (referred to as back-ends) which perform computations in parallel. The issue with this topology, however, is that the front-end node can easily become overwhelmed by the amount of data being sent back and forth from the back-end nodes. A solution to this problem is to reduce the number of back-nodes in direct communication with the front-end node. Achieving this solution entails creating a Tree-Based Overlay Network, where the front-end node represents the root of the tree and the back-end nodes represent the leaves. The intermediate vertices of the tree are nodes in the environment that relay information back and forth between the front-end and backends. These intermediate nodes can also perform data aggregation and filtering to reduce, optimize, and synchronize information sent to the front-end, further distributing (and thus reducing on the front-end) computational and bandwidth loads. Though this solution is typically employed in the context of HPC tools (performance profilers, parallel debuggers, system monitors, and system administration tools), there are also several non-tool uses, including commonly-used algorithms for which Tree-Based Overlay Networks are well-suited.

Mandy Cortez
New Mexico Highlands University
HPC-1
Mentor: Robert Kelsey

Presentation Title: Searching the World Wide Web (WWW) with Efficiency

Presentation Abstract: As the World Wide Web (WWW) is increasing in size so is the amount of information that is available. With the availability of so much information the issue of finding the most pertinent information from WWW search results can be difficult. Data mining, which is the process of analyzing data to identify patterns and relationships, is one technique known to optimize search results. To address this issue, the data mining technique of document clustering is used to group together documents that have content similarities. This was done by building a web document data set to test two different clustering algorithms. The first algorithm was an overlap clustering algorithm and the second was the K-Means algorithm. Through testing with several different search terms at different thresholds the results showed that the document clustering algorithms did create clusters of documents with similar content. It also showed that applying particular thresholds increases the precision of the cluster content. With more research and testing this technique can be used in Web searching to increase the accuracy and accessibility for obtaining documents pertaining to the information being searched.

Ekaterina Davydenko, University of New Mexico,
HPC-5
Mentor: Hsing-Bung Chen

Presentation Title: Xen Virtualization Scaling and Enterprise Environment

Presentation Abstract: The purpose of this project is to scale a Linux cluster from a testing environment to a full scale enterprise. We are currently working with a cluster of ten nodes, one as the master control node where all of our main services dwell, such as DHCP, DNS, LDAP, NFS, and Nagios (a monitoring application). Each of these machines currently runs two AMD Opteron 250 CPU's accompanied by two gigabytes of RAM. The main purpose of this cluster is to serve as an entity to run MPI programs including benchmarking software, then to compare results with our fellow teams to see who achieved the best results. Our particular assignment is to use Xen virtualization software to simulate a larger cluster; we are aiming to simulate around a one hundred node super cluster. We are planning on upgrading the hardware configuration of the machines from originally installed two gigabytes of RAM, to four gigabytes of RAM per node to ensure that we have enough system resources available to support the amount of virtual nodes that we are planning on implementing. This project purpose is to see how virtual nodes effect the scaling capabilities of these benchmark software applications across the cluster. Do modern day super clusters really need to be as massive as they are, or can we use the aid of virtualization to minimize the amount purchased nodes? This method of virtualization can be very useful prior to purchase when planning a cluster implementation; with this method you can test your targeted applications to see just how many nodes you actually need. That was from an economic point of view, and another aspect of this research is to see exactly where these applications reach their performance threshold. Exactly when does a certain function reach its peak performance? After how many added nodes performance of application doesn't change? Tests also will include the scalability of Xen itself, meaning how Xen scales with different types of hardware, and when it starts to lack performance due to lack of hardware resources. All this is applicable when determining software we are hoping to provide an efficient aspect of testing prior to cluster implementation.

Julius Jackson
Central State University
IST-APPS3
Mentor: Justin Tozer

Presentation Title: Writing and Executing Test Cases in the Waste Compliance and Tracking System

Presentation Abstract: Los Alamos National Laboratory (LANL) generates transuranic waste that must complete a complex certification for disposal at Waste Isolation Pilot Plant. The Waste Compliance and Tracking System (WCATS) is a software application used for managing the treatment, storage, and disposal of transuranic waste at LANL. In order for WCATS to be certified, the user interface, functionality it provides, and the data it produces must be without error. Testing, which is required by the software quality assurance process, helps achieve this goal. For example, discrepancies between the design of a component and its intended outcome, or better ways to simplify the use of WCATS have been found through testing. This allows the necessary changes to be made in order to achieve a better final product. This presentation will review how the test processes for WCATS were created, executed, how feedback was provided, and the benefits testing provides for developing a certified system for managing transuranic waste.

Andrew Konwinski
University of California, Berkeley
HPC-5
Mentor: Meghan Quist

Presentation Title: A close look at large parallel work loads

Presentation Abstract: There is strong demand for I/O tracing in High Performance Computing (HPC) for several reasons. First, it enables in-depth workload analysis and performance tuning. Second, it facilitates collaboration within and between governmental, industrial, and academic institutions by enabling the generation of replayable I/O workloads which can be easily distributed and anonymized if necessary to protect confidential or sensitive information. As a response to the demand for I/O tracing, various means of trace generation have been explored. We first survey several tracing mechanisms from system I/O call interposition to stackable file systems. Examples include TraceFS (Stony Brook U), //TRACE (CMU), and MPItrace (LANL). We then analyze and compare the performance of each tool, in terms of tracing time overhead, the flexibility of the data we are able to capture, and trace replay fidelity. We use a number of synthetic and real workloads, testing at varying levels of I/O behavior, including file size, process-to-file ratio, and strided/non-strided

Caleb Morse
University of New Mexico
CTN-4:
Mentor: Susan Coulter

Presentation Title: Advance Health Monitoring of Computer Clusters

Presentation Abstract: As the number of nodes and processors in a cluster grows, its interoperability and networking become more complex. This complexity drastically increases the amount of system errors and decreases performance. To ensure the accuracy and speed of a cluster, it is important the system be monitored and managed in an efficient and effective manor. Monitoring tools must quickly and correctly recognize performance degradation in clusters without requiring excessive system resources. They must also communicate with system administrators promptly to avoid smaller issues turning into systemwide problems. Our solution incorporated Nagios, a monitoring software, and Cacti, a graphing program, along with homegrown monitoring processes to track a small cluster's performance. Failures and delays will be injected into the system, such as unnecessary daemons and network errors, to ensure monitoring tools are providing swift and correct 07data.

Milo Polte
Carnegie Mellon University
HPC-5
Mentor: John Bent

Presentation Title: Multidimensional Extensions to a Distributed Filesystem

Presentation Abstract: Traditional file systems index files along a single dimension, that of the path and filename, but as we approach the age of peta-scale high performance computing clusters, the number of files in our storage systems will begin to outstrip our ability to organize and search using this single dimensional approach. To support modern applications such as autonomous sensor networks, a multidimensional indexing approach is needed to allow applications and users to tag files with attributes efficiently and filter files based on these tags. Traditional solutions to the problem have been to embed metadata information in the file name (which is limited and inefficient search) or to store file tag information in a separate database system (which makes maintaining coherence is nontrivial and requires the behavior of users and applications to be modified to use a database interface rather than the more familiar and universal POSIX file system API). In this project we add a multidimensional extension to the Parallel Virtual File System to resolve these issues. The extension provides efficient tagging of files and Structured Query Language-style querying. Unlike a separate database approach, the tighter integration allows tagging and querying to be accessible through normal file system commands such as 'ls' and 'mkdir', and coherence is tight. We will evaluate the overhead imposed by the extension, and measure the trade-offs between time-till-coherence and performance.

Scott Ramsey
University of Illinois, Urbana-Champaign
X-1
Mentor: James Kamm

Presentation Title: The Eigenvalue Problem of Reflected Shock Waves Generated by Symmetric Implosions

Presentation Abstract: It has been noted that G. Guderley's self-similar analysis of a converging shock wave can be extended into the positive time domain; that is, the shock wave is physically observed to "reflect" about an axis or point of symmetry and propagate outwards into the once-perturbed gas. It will be demonstrated the resultant motion and flow behind the reflected shock wave remains self-similar, with the previously-determined "similarity exponent" and an initially unknown reflected trajectory multiplier (a second nonlinear eigenvalue) as key parameters. The identification of relevant boundary conditions and the determination of the trajectory multiplier will constitute full solution of the reflected shock wave problem; physical flow variables can be subsequently recovered through the use of appropriate similarity transformations and compared to results derived from existing codes

Tiberiu Stan
University of California, Santa Barbara
IST APPS3
Mentor: Justin Tozer

Presentation Title: Automation of Authorization Requirements for Radioactive Waste Compliance

Presentation Abstract: Each year the Los Alamos National Laboratory gets audited for agreement with hazardous waste procedures; and failure to obey the regulations results in fines, penalties, and a loss of public confidence. The Waste Compliance and Tracking System (WCATS) uses the concepts of task, task approval, and task execution to restrict actions that would violate requirements all the while giving users the freedom of customizing their procedures. WCATS can evaluate hundreds of restrictions impacted by a single waste transfer, shipment, or processing operation which would be difficult for a human to enforce without making mistakes. Examples of requirements include Material at Risk (MAR) limits for radioactive waste, RCRA less than 90-day area regulations, process limits for Pu-239 fissile gram equivalents (FGE), container weight/volume limits, authorization to generate waste, and correct assignment of EPA Codes. The system's ability to manage waste processes, verify compliance with all regulations, and keep permanent records of each attempted task execution allows operations personnel to sleep without the fear of losing their job.

Henry Talachy
University of New Mexico
IST APPS3
Mentor: Justin Tozer

Presentation Title: Implementing Reporting Capabilities in LANL's Waste Compliance and Tracking System

Presentation Abstract: The Waste Compliance and Tracking System, or WCATS, is a Java and Oracle based three-tier computing system that is designed to better handle the oversight of radioactive waste generated at the laboratory. The system is capable of managing waste from its point of generation to its ultimate disposal. As WCATS is a very complex system, reports are fundamental for the presentation of significant information to users in a manner that is comprehensive, intuitive, and readable. Reports can be used for many things such as regulatory reference documentation, waste inventory reports, and hardcopies of relevant information to vital application subsystems. While there are many types of reporting systems, this presentation will focus on the technologies and products in WCATS, and how they are implemented in the system.

Kelcey L. Tietjen
The George Washington University
CTN-5
Mentor: Kersti Rock

Presentation Title: Searching for Rootkits with Windows Memory Analysis using EnCase

Presentation Abstract: With the prevalence of rootkits as being the new subterfuge vector for hacker's new tools and techniques need to be developed to detect these pieces of malware. Rootkits are especially deceptive because they hide what the attacker is doing on the system evading detection even from the most seasoned system administrator. One of the harder to detect rootkits is one that is located with in windows memory and leaves no trace of itself on the hard drive and is only detectable in a physical dump of memory. Windows memory analysis does not stop at finding malware but can also be utilized in other forensic investigations aiding in problems with encrypted data areas and waste fraud and abuse cases. Discussion of Windows processes data structure will be detailed to give background on how to find these rootkits and other processes in a physical memory dump. The tools that were developed and will be discussed in this presentation will go over how to obtain physical memory dumps over the network using EnCase Enterprise and how to detect the memory rootkits and other processes on the machine that might not be detectable otherwise.

EARTH & SPACE SCIENCE

Jesse Canfield
New Mexico State University
EES-2
Mentor: Rodman Linn

Presentation Title: Importance of Three-Dimensional Aspects in Wildfire Behavior

Presentation Abstract: The purpose of this research was to investigate the importance of the three-dimensional (3-D) aspects of wildland fire behavior and determine if a two dimensional (2-D) representation (vertical slice perpendicular to a long fire line) can be used to capture the critical phenomena that drive wildfires forward. HIGRAD/FIRETEC, a numerical, coupled atmosphere-fire model, was used to perform a series of grassfires designed to address these issues. HIGRAD/FIRETEC was used to perform a series of simulations of infinitely long (but periodic) fire lines with the same number of cells and resolution in the x (streamwise) and z (vertical) direction, but the number of cells in the y (crosswind) direction is varied between 40 cells and 1 cell. The resolution in the x and y directions is held fixed at 2 m and the vertical resolution is 1.5 m near the ground but stretches upward. The computational domain was 2560 (m) in the downwind direction and 615 (m) in the vertical direction. Each domain, geometry, had ambient wind velocities ranging from 1 to 18 (m s^{-1}). Fire spread rate, fire line geometry, heat transfer, and turbulence were compared for each wind speed case. These properties evolve differently when only 1 cell in the y direction is used since this becomes a 2-D simulation. There is a threshold of domain width where below that width the critical 3-D processes cannot be resolved and the fire behavior becomes more like that of a 2-D infinitely thin plume (like a plume in a fluid between two pieces of glass.)

Giuseppe Colantuono
Florida State
CCS-2
Mentor: Wilbert Weijer

Presentation Title: Topographically intensified Rossby basin modes in a two layer numerical model

Presentation Abstract: Observations show several modes of large-scale variability in the Argentine Basin. A barotropic numerical model has identified only some of these as Rossby basin modes, trapped by the "Zapiola Rise" seamount. We therefore employ a two layer model to mimic the "real ocean" stratified dynamics. Using an eigenvalue solver we have determined the normal modes of the basin, and studied their sensitivity with respect to some key physical quantities. The modes found with the two layer model belong to two classes that resemble, respectively, the properly defined barotropic and baroclinic modes of a two layer fluid in the flat bottom case. We have examined the sensitivity of the barotropic-like modes with respect to layers density difference and interface depth; their period is monotonically increasing, both with respect to a shoaling interface and a decreasing layers density difference. The spatial patterns of the modes seem, on the contrary, virtually insensitive respect to the above parameters and also very close to the ones obtained with the barotropic model. Nonetheless, the changes are too small to account for the discrepancy between a 25-day mode from observations and a 31- day normal mode from our shallow-water model.

Jonathan Gramann
Texas A&M University
EES-6
Mentor: Manvendra Dubey

Presentation Title: Atmospheric Aerosol and Cloud Interactions

Presentation Abstract: Human induced climate change is an issue that has come to the forefront of environmental policy in recent years. A significant quantity of research has already been undertaken in an effort to answer the questions "how much?" and "how fast?" But, the variety of answers is indication of how much more research there is still to do. The latest IPCC assessment lists particulate matter, or aerosols, as one of the least understood mechanisms of radiative forcing. Aerosols, in fact, have two effects. The first, the direct effect, is the scattering and absorption of solar radiation as it passes through the atmosphere, which acts to increase Earth's albedo as well as increase absorbed solar radiation. Research suggests that this creates a net radiative cooling effect. The indirect effect results from the interaction of aerosols with water vapor to form larger and longerlived clouds, dramatically influencing planetary albedo. Our research focused on these effects and analyzed data from two campaigns that utilized data gathered from airplanes. The first campaign was undertaken in September 2006 over Houston, and the second in June 2007 over Oklahoma City. A photoacoustic instrument was used, which gathers aerosols in a chamber and heats them with a laser; this produces an acoustic signal due to the heating of particles and the expansion of air. From this instrument and others, we gathered data about the scattering and absorption efficiencies of the aerosol sample. We observed an overall trend for scattering, as well as the ratio of scattering to overall extinction, decreasing with height through the boundary layer, leading to our hypothesis that clouds were selectively scavenging or activating scattering aerosols rather than absorbing aerosols.

Sarah Nelson
New Mexico State University
EES-2
Mentor: Rod Linn

Presentation Title: Two-Dimensional Modeling of a Fire or Plume in a Cross Flow and its Limitations

Presentation Abstract: For a variety of reasons, researchers and practitioners are interested in understanding fire and plume behavior in a crosswind through numerical modeling. Unfortunately, simulating a fully three-dimensional fire or plume is sometimes computationally prohibitive. One postulated approach would be to consider an infinitely long fire line in a two-dimensional vertical planar context. With this approach, it is possible to examine some interactions between the wind and a buoyant plume from a fire or other heat source. But the question remains: Is simulating a long fire or heated plume with a vertical plane perpendicular to the length of the heat source an effective and valuable way of understanding the physics of a real plume? A twodimensional computational fluid dynamics code has been written with a heat source at the bottom of the domain to view and analyze the plume rise at different wind speeds. An area with a specified heat source represents the area on the ground that is on fire, assuming this simulation is a vertical slice of a wildfire. By running this code and visualizing the results, we can examine how the plume rise looks as time progresses. However, had a third dimension been simulated in this code, we would have seen that a fire is not homogeneous in that third dimension. It in fact has fingers and lobes, so the interaction between the buoyant plume and the wind has definite three-dimensional behaviors. The result is that some of the wind would simply blow between those fingers of the plume and not affect the plume rise. Another problem to take into account is that when a fire is ignited and it moves along, it forms an arc rather than staying in a straight line. The two dimensional code does not show this characteristic either. Because of these two points, we can see that modeling fires or strongly buoyant plumes in only two dimensions may be misleading since it leaves out potentially important physics.

Jeremy Sauer
Florida State University
EES-2
Mentor: Rodman Linn

Presentation Title: Impact of Multiple Fuels Representation in Wildfire Modeling

Presentation Abstract: Firetec/Higrad is a physics based wildfire model developed at LANL. The model couples a 3-d fully compressible atmospheric dynamics component (HIGRAD) with a physics based combustion component (FIRETEC) to provide a more detailed look at wildfire dynamics than current operational models provide. Most operational models are based on empirical formulae and are optimized to provide estimates of fire spread rate and other characteristics important to managers during containment of existing fires. FIRETEC/HIGRAD allows researchers to study the complex phenomena of wildfires in much greater detail with the intention of using these model results to improve the empirical relationships of the operational models. This work presents an additional approach that extends the physical representation of wildland fuels in the FIRETEC/HIGRAD model. Previously fuel characteristics within a cell were assumed to be an averaged quantity over the cell volume, thus all bulk density, moisture content, sizescale, etc. were assumed to be homogeneously distributed over a cell volume. The multiple fuel types approach allows FIRETEC to describe some of the unresolved heterogeneity by treating the fuel bed as a mixture of fuels with potentially different surface to volume ratios, moisture contents, packing ratios, etc.. This adds the potential of describing the processes that were not possible before, such as burning dry thin fuels providing enough heat to ignite thicker more moist fuels in the same cell. Calculations of convective heat exchange, radiation emission/absorption, fuel reaction rate, and fuel induced drag are all calculated for each fuel type within a cell. This work describes the implementation of the multiple fuel types approach and presents model results from several idealized scenarios to illustrate the impacts of increased accuracy in fuel representation.

ENGINEERING

Nathan Barnett
Oregon State University
X-3
Mentor: Forrest Brown

Presentation Title: One Group Transport Cross Section Generation for MCNP

Presentation Abstract: One group problem scan be invaluable in the transport world. They can be used to match an existing code to analytical answers, match a new code to an existing code, or even develop new methods. MCNP is a widely used and trusted transport code which has the capability of running multi-group and thus one-group problems. ONEGXS was developed to convert simple, user provide data, to the required ACE form at for use in one-group M CN P calculations. Results from MCNP using data provided by ONEGXS will match analytical results for both isotropic scattering and linearly anisotropic. However, if the scattering is highly forward or backward peaked, here the absolute value of the average cosine of the scattering angle is greater than 1/3,answers will be skewed. While several methods exist for constructing the scattering function in these extreme conditions, none stand out as more correct than any of the others. ONEGXS uses a constant function over a portion of the scattering range, chosen so that the first moment is preserved.

Alberto Canabal
New Mexico State University
AOT-MDE
Mentor: Tsuyoshi Tajima

Presentation Title: Coupled Thermal-Electromagnetic Model for the Analysis of Multilayer-Coated Superconducting Accelerating Structures

Presentation Abstract: Multilayer coated accelerating structures might be able to push the limit of accelerating gradient for superconducting RF cavities and give some benefits to dielectric cavities. A numerical study of the thermal quench in multilayers of superconductors will be presented, where each additional superconducting layer has a thickness less than their corresponding London penetration depth. The goal is to characterize a microwave pulse incident upon a multilayer-coated accelerating structure. A coupled thermal-electromagnetic model will be presented, where the electromagnetic and thermal analyses will be performed in the frequency and time domains, respectively. The detailed description of the model and simulation will be shown during the talk with some results if available.

Adam Davis
North Carolina State University
AET-2
Mentor: Drew E. Kornreich

Presentation Title: A New Analytical Formula For Photon Buildup Factors In Dual Layer Shields

Presentation Abstract: In radiation protection, photon buildup factors provide an easy method for calculating dose response after various shielding configurations as well as information about the behavior of radiation in these configurations. Though many situations call for multi-layer shields, few data bases and derived analytical formulas for photon buildup in multi-layer shields exist. This research develops an analytical fit for dual layer shields of various materials, and provides insight into the effects of material order and thickness on photon buildup factors in such shields by examining flux data calculated in the discrete-ordinates code Partisn and benchmarked in selected cases with the Monte Carlo code MCNP5.

David Geb
University of California, Los Angeles
AET-5
Mentor: Torsten Staab

Presentation Title: Practical DNA-Based Clinical Diagnostics

Presentation Abstract: The development of a disposable test cartridge for DNA-based clinical diagnostics will afford a better alternative to current protein-based tests. DNA-based clinical diagnostics is significantly more accurate than the protein-based alternative. Moreover, a cheap, effective, disposable test cartridge will allow this technology to be accessible to more patients. The development of this test cartridge involves designing, prototyping, assembling, and testing its mechanical components. After the completion of the project, a user-friendly, affordable, and accurate device will be the result. Its technology will provide a solution for clinical diagnostics in physician offices worldwide.

William Godoy
University at Buffalo
X-4
Mentor: Mark Carrara

Presentation Title: Modeling radiation heat transfer in multiphase flows

Presentation Abstract: A deterministic approach is developed to model the coupling of radiation and multiphase flows for a three-dimensional domain. A formal averaging procedure is applied to model the mass and momentum conservation of a multiphase flow and the energy equation is coupled with the influence of the radiating system. A correlated-k approach is incorporated to relax the complicated spectral dependence of the radiative properties of the medium composed of mainly water droplets and gases and a deterministic discrete oridinates method (DOM) is applied to solve the radiative field at every time step. Results show the importance of radiation in the overall mass and energy transport and vast application of this model can be further explored for cases such as: explosions, reacting systems and fire environments.

Lee Harding
University of New Mexico
X-3
Mentor: Forrest Brown

Presentation Title: Electron Soft Collisions Using Moment Preserving Models in MCNP

Presentation Abstract: A new method for sampling energy-loss straggling in MCNP has been implemented, using moment preserving models. These models use the moments of the Møller differential cross section (D CS)to create an approximate DCS. The approximate DCS is created by preserving the moments Møller DCS exactly. While the Møller DCS is accurate for hard collisions for incident electrons, it does not account for effects due to binding energy (soft collisions). To account for soft collisions the Bethe-Bloch treatment for stopping power is used to generate a straight forward continuous slowing down approximation for benchmark calculations, and a modified Bethe-Bloch stopping power can be used in combination with the stopping power from the Møller DCS in the moment preserving model as data for the moment preserving DCS to accurately model soft collisions. This presentation will briefly describe the moment preserving model, incorporation of soft collisions and comparisons of the moment preserving model to the current model used in MCNP.

Jason Jaworski
Purdue University
ISR-1
Mentor: Tom Prettyman

Presentation Title: Optimization of CdZnTe Semiconductor Anode Electrodes Using Gallus

Presentation Abstract: Steady advances in crystal growth have led to a significant increase in the size of CdZnTe single-crystals available for gamma ray spectroscopy. Spectrometers are now being constructed using crystals > 2 cm3 in volume, some of which will yield detection efficiencies comparable to scintillators used in hand-held, nuclear material measurement applications. As in previous efforts, an electrode pattern and read-out technique must be developed and optimized in order to effectively compensate for carrier trapping and other limiting factors, such as surface effects and variations in bulk electronic properties. Our goal is to achieve a pulse height resolution better than 3% full-width-at-half-maximum (FWHM) at 662 keV for a 6 cm3 crystal, which will significantly improve our capabilities for isotope identification. To support this effort, we have developed a three-dimensional code, called GALLUS, which models waveforms and pulse height spectra for complex anode structures, such as coplanar grids and pixel-based designs. This code package in conjunction with an IDL program that generates the input for GALLUS, including grid parameters and boundary conditions for specific anode designs, will be utilized to find an optimal coplanar anode design. A new program will be written which employs the downhill simplex method in several variables to optimize the shape of the anode structure. The figure of merit tested by the optimization program will be a measure of the difference between the collecting and non-collecting anode weighting potentials, which is a major factor that determines the resolution of the detector. After the parameters are optimized, a Monte Carlo simulation will be run to estimate the pulse height spectra. A review of Gallus and details of the optimization code are described.

Saryu Jindal
University of California, Davis
MST
Mentor: Richard Hoagland

Presentation Title: Structure and phase transformations of an asymmetric $\Sigma 11$ grain boundary in copper at high temperatures

Presentation Abstract: Grain boundaries are internal interfaces formed when two crystal surfaces brought together are misoriented relative to each other. These are places where atoms form unique arrangements as compared to the atomic configuration in the adjacent lattices. Five macroscopic degrees of freedom are required to specify the interface between two crystals. In addition to this, there are three microscopic degrees of freedom that correspond to the shear displacement vector. In this project, seven degrees of freedom (5 macroscopic, and two microscopic (D_x and D_z)) were used to specify an asymmetric $\Sigma 11$ tilt boundary. Various structures, or metastable states, for the grain boundary were found corresponding to distinct microscopic degrees of freedom. To systematically study these structures a γ surface (which describes the variation of energy with shear displacement vector) was constructed for the asymmetric $\Sigma 11$ tilt boundary in copper at 0 K using static molecular dynamics. In addition to the single configurational states found at 0 K, at finite temperature multiple states may coexist in the grain boundary. Different points on the gamma surface (corresponding to different structures of the boundary) are taken as initial configurations and annealed to different temperatures for a certain amount of time. The resulting equilibrium structures are studied and compared to the initial structures.

Brian Kienitz
Case Western Reserve University
MPA-11
Mentor: Bryan Pivovar

Presentation Title: A half cell model of steady state PEM fuel cell performance degradation under contamination by foreign cationic species

Presentation Abstract: When cationic impurities, such as alkaline metal ions, are present in a polymer electrolyte membrane fuel cell (PEMFC) the performance of the PEMFC can be significantly reduced. These contaminants can enter the membrane and catalyst layers from other fuel cell components, feed streams or from the external environment. Cations can replace protons in the membrane in accord with normal ion exchange processes, as they, in general, have a higher affinity than protons for the sulfonic acid group sites in the polymer electrolyte. This presentation will discuss ongoing modeling and experimentation effort to study the effects of cationic contaminants on PEMFC performance. This model accounts for the transport and reaction of protons and oxygen in the cathode electrode, and mass transport in the cathode side gas diffusion layer (GDL). It does not consider the anode half cell and it assumes the flux of cationic contaminants is negligibly small compared to the flux of protons across the membrane. Results show that cationic contaminants will always be more concentrated at the cathode side of the fuel cell when any current is drawn. At the point of maximum current the fraction of cationic impurities occupying acid sites is zero. The catalyst layer is also affected by the concentration profile of cations in the cell since it is partially made of polymer electrolyte. The reduced proton concentrations lower the reaction rate which in turn increases over-potentials. This model gives insight into the main observed effects of fuel cells operating with cationic contamination. The model explains how cationic contamination can lead to the observed changes in polarization and limiting current. Potentially this model can be used to aid in the diagnostics of contaminated fuel cells and the design of future fuel cell components.

Alexandria Marchi
New Mexico Institute of Mining and Technology
W-7
Mentor: Michael Smith

Presentation Title: Complexity of Acoustic Emission Spectra during In-process Monitoring of Pinch Welds

Presentation Abstract: Solid-state resistance closure welds (pinch welds) are used to seal tritium containing gas transfer systems. Acoustic emission (AE) monitoring has been suggested as an in-process, non-destructive evaluation (NDE) of pinch welds. This discussion considers some of the factors that may contribute to the observed AE spectra, specifically machine noise, mechanical squeezing, and any energy contributions from applied voltage. AE contributions from squeezing and un-squeezing the electrodes were minimal and did not contribute to the complexity of AE spectra. However, a considerable affect on the AE spectra was observed by varying the number of applied weld cycles. The frequency content of AE events, during the on-heating and on-cooling portions of the AE signature, was directly related to the number of weld cycles. The complex nature of the on-cooling section was demonstrated mathematically using Fast Fourier Transforms (FFT) and Principal Components Analysis (PCA). The number of AE events produced during on-heating consistently increased with current thus, analysis was not deemed important. Our results are interpreted in light of the grain growth hypothesis first proposed by Smith and Hartman (2005).

Matthew Marzano
University of Florida
ISR-1
Mentor: Tom Prettyman

Presentation Title: Internal Electric Field Mapping of CZT Using Pockels Birefringence

Presentation Abstract: Cadmium zinc telluride (CZT) crystals are used for gamma ray spectroscopy of radioactive materials for Homeland Defense Applications. Improvements in crystal growth techniques have led to significant increases in the size of single crystals, resulting in increased efficiency needed for isotope identification. Electronic characterization is needed in order to assess performance and optimize electrode design. A uniform internal electric field is desired to achieve optimal performance as a gamma-ray detector. When subject to an applied electric field, CZT displays a linear electro-optic effect, known as the Pockels effect. Pockels effect provides us with a unique method of measuring the internal electric field within the crystal. An ideal CZT crystal (free from defects) is transparent to IR light. Mapping the internal electric field involves the illumination of the crystal with linearly polarized light and an applied bias. The images are captured by an InGaAs IR camera, and the light intensities are determined. From the measured light intensity, the internal electric field can be determined. We found that the electric field is often non-uniform, which may result from the production of free carriers by photo-excitation. Alpha particle induced charge measurements will be carried out to verify the observed variation in the electric field. Until now, similar experiments have analyzed crystals with planar electrodes. The crystal we will be looking at will have a coplanar grid anode. Preliminary investigations were made at Fisk University and will be reported along with the experimental setup under development at Los Alamos National Laboratory.

Brian R Nease
University of New Mexico
X-3
Mentor: Forrest Brown

Presentation Title: Implementing the Coarse Mesh Method into MCNP for Dominance Ratio Calculation

Presentation Abstract: Recently, a robust method of determining the dominance ratio (Coarse Mesh Method) was developed for iterated source Monte Carlo (MC) methods. The objective of this method was to correctly evaluate the dominance ratio using time series techniques in a completely automated fashion, without requiring specific knowledge of transport theory or time series analysis from the user. In this work, CMM was integrated into MCNP and tested against several benchmarked problems. Since MCNP is a production code, there is a strong desire to reduce memory usage and improve algorithm efficiency with any new methods introduced. With these constrains in mind, CMM was introduced using a two-bin scheme. CMM performed very well (due to the symmetric nature of most problems), though a bin scheme matching the problem dimensions would be more advantageous to ensure that the largest eigenmode of the noise propagation matrix does not cancel out for any particular problem. The difficulties with implementing this larger bin scheme will be discussed, followed by the results of CMM against several test problems in MCNP.

Andrew T. Nelson
University of Wisconsin
MST-8
Mentors: Stuart Maloy, Dave Dombrowski

Presentation Title: Development of Diffusion Bonding Parameters for HT9-W and HT9-Ta

Presentation Abstract: The Materials Test Station (MTS) is currently being investigated as an upgrade to LANSCE that will allow researchers the unique ability to perform nuclear fuel and structural material irradiations in a purely fast neutron flux, similar to conditions in the proposed GNEP reactor suite. This flux is generated by means of colliding protons with a tungsten or tantalum spallation target to produce neutrons in the MeV spectrum. Due to the oxygen affinity possessed by refractory metals and their embrittlement under neutron irradiation at the proposed operating conditions, the target will require cladding in a stainless steel. Ferritic-martensitic stainless steels (e.g. HT-9) are preferred to traditional austenitics in neutron environments due to their extended swelling resistance at 400 C. Bonding of HT9 to the target material will prove vital to the MTS design not only to maintain tungsten structural integrity, but also ensure maximum thermal evacuation in the even of a loss of coolant accident. Given this vital constraint, a purely mechanical bond will not suffice as gaps as small as a thousandth of an inch will greatly increase the thermal resistance. Diffusion bonding is successfully used in specialty applications to join dissimilar materials by applying moderate pressures at elevated temperatures to produce a bond within the parent materials without the need for a liquid interface. For MTS development, a test matrix of three temperature-pressure-time states will be used to bond a series of HT9-W and HT9-Ta interfaces with different nickel-based coatings applied to the HT9 to suppress oxide influence. Following bonding, the parent material is analyzed using optical microscopy and compared with the as-received condition and the interface inspected for voids or other unexpected phenomena. Scanning electron microscopy (SEM) energy-dispersive spectrometry (EDS) techniques are relied upon to quantify diffusion of the steel constituents into the target (and vice versa) to determine the thickness of the diffusion zone. Finally, flash diffusivity is combined with differential scanning calorimetry (DSC) to generate thermal conductivity values for the bond to assist in MTS design.

Clell Soloman
Kansas State University
X-3
Mentor: Avneet Sood

Presentation Title: A Linear Tally Combination Addition to MCNP

Presentation Abstract: A linear tally combination feature has been added to MCNP5. Implemented as primarily stand-alone module, this new feature provides the user the capability of combining tallies with user specified multiplier values. Additionally, this tally combination has been tied into the weight window generator such that weight windows may be generated for the linear combination. This presentation will discus the application of the linear tally combination to test problem sand weight window generation and the computational gains observed.

MATERIAL SCIENCE

Alyson Niemeyer
University of Florida
MPA-11
Mentor: Brian Crone

Presentation Title: High Quantum Efficiency Polymer Photoconductors Using Interdigitated Electrodes

Presentation Abstract: In this study we investigate photoconductivity in interdigitated lateral photoconductors with aluminum contacts, and a poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylene-vinylene] [MEH-PPV] / {6}-1-(3-(methoxycarbonyl) propyl)-{5}-1-phenyl-[6,6]-C61 [PCBM] blend as the active layer. We demonstrate quantum efficiencies over 70% in 5 _m devices. The absorption in the MEH-PPV/PCBM films can be fit with a linear sum of the absorption of MEH-PPV and PCBM films. The quantum efficiency spectra follows the absorbance spectra for films with optical densities <1. The quantum efficiency is a monotonically increasing function of applied field. The field dependence can be explained with a modified Onsager model for charge dissociation. Experiments using a pulsed light source were also performed and the results are reported.

MATHEMATICS

Julianne Coxe
James Madison University
LANSCE-LC
Mentor: Thomas Proffen

Presentation Title: How many licks does it take to get to the center of a tootsie roll pop? -OR- How many hours does it take to model the local atomic structure of a sample? Two. Four.... Six.....Six!

Presentation Abstract: NPDF at LANSCE uses neutrons from the proton beam to determine the local atomic structure of samples placed in the machine. The experiment currently has neither a generic time frame in which to measure, nor a set of requirements after which to stop. Since neutrons are a precious commodity, this project has been established to minimize the number of unused or wasted neutrons by finding the point in time when the output does not get any better. Who would not want to be able to do two experiments within the time of one? The areas that make this a difficult problem to solve are the Fourier transform to obtain the atomic pair distribution function and the noise that is accumulated in the background of each run. Although it is pointless to try to measure to the point of no noise, it is believed that there will be a point after which the decrease in noise will not validate the time spent. This project is on a mission to find this time or to find that it does not exist, since either would be helpful. The data analyzed was that of silicon and glass, whose atomic structures are already known. Statistical criteria have been calculated from the scattering data. The optimal time will be achieved when a certain percentage of these criteria have been attained and measuring any longer to gather any others would not be worth the time spent. In the future, a program will be installed into NPDF's computer to calculate these parameters and to tell the experiment to halt the experiment.

Humberto C. Godinez
Portland State University
T-7
Mentor: David Moulton

Presentation Title: Sensitivity Analysis in a New Cloud Resolving Aerosol Model

Presentation Abstract: Due to the computational power now available, more realistic mathematical models can be used to describe various physical phenomena. As the models improve new parameters are being introduced whose values are not accurately known, and may lack a strong connection to first principles. Determining the values as accurately as possible of all parameters can be a challenging and expensive endeavor, hence, identifying the most influential parameters is of great importance. Sensitivity analysis enables the identification of the most significant parameters in a model, thus providing valuable insight into which of these should be accurately determined. The objective of our research is to perform a forward and adjoint sensitivity analysis, as well as to study other aspects of uncertainty quantification, in a new cloud resolving aerosol model. Sensitivity of the solution to the models various parameters, as well as aspects of its discretization, will be tested and the most relevant ones identified. We will implement this sensitivity analysis in an MPI-based parallel code for the cloud resolving aerosol model. This work will contribute to current research on sensitivity analysis and uncertainty quantification in new high-resolution models of cloud aerosols. In addition, it will bring critical insight into the influence of numerical discretization errors on the predictability of these models.

NON-TECHNICAL

Charles Streeper
Monterey Institute
N-2
Mentor: Cristy Abeyta

Presentation Title: Nefarious Uses of Radioactive Materials

Presentation Abstract: The November 2006 death of Alexander Litvinenko through the ingestion of 210Po (polonium-210) has reignited the debate concerning the possibility of the future malicious use of radioactive materials. However, before making any assumptions about this incident based upon the media frenzy surrounding the case, it would be prudent to look at past incidents in order to put it in perspective. This paper looks at past incidents of misuse of radioisotopes in order to look at the Litvinenko case through a historic lens. In the course of this research, several moderately restricted databases and one open-source document were discovered; several conclusions have been provided on the effectiveness of these databases. Data provided by the International Atomic Energy's Illicit Trafficking Database (ITDB), the Database on Nuclear Smuggling, Theft and Orphan Radiation Sources (DSTO), the Center for Nonproliferation Studies' (CNS) WMD Terrorism and CBRN Incident and Response Databases, Johnston's Archive's Database of Radiological Incidents and Related Events and from a research paper giving a global chronology of radioactive attacks were used to compile a general background on past malevolent uses of radioisotopes.

PHYSICS

Sean R. Brannon
Dickinson College
T-4
Mentor: Yongho Kim

Presentation Title: Non-thermal Plasma Effects on Hydrogasification of Coal

Presentation Abstract: As oil reserves continue to be depleted and energy prices continue to rise, the search for viable alternative energy sources is taking on an increasing importance. One such alternative energy source is hydrogen and methane fuel produced by coal gasification. LANL has developed the ZEC (Zero Emission Coal) concept, which utilizes methane produced by the hydrogasification reaction. ZEC comes with several benefits, including the plentiful supply of coal (enough for more than 100 years even assuming increasing rates of consumption), potential energy efficiencies of >65% (as compared with <35% for traditional coal-fired plants), and the possibility for zero carbon emissions. However, the technology is still mostly undeveloped commercially and needs significant improvement before it will become economically viable. In particular, hydrogasification reactions currently proceed far too slowly, and accelerating the reaction with traditional catalysts is not possible due to the highly abrasive environment inside the reactor. Thus, the key to making coal gasification a practical alternative is to increase the rate of reaction without using traditional catalysts. Our project involved investigating how a non-thermal plasma might be used in a catalytic role. Specifically, our method is to partially ionize a small fraction of the coal and reactant gases, creating chemically active species (CAS) which can interact with the feedstock in the reactor, increasing the rate of reaction and the percentage of feedstock conversion and possibly allowing us to decrease the temperature and pressure in the reactor. To study these effects, we took a two-pronged approach: first, we modeled the reactions computationally by using ELENDIF code to study the creation of CAS by the plasma and HSC code to examine the effect of the CAS on the reaction for given temperature and pressure conditions; and second, we performed experimental tests to measure the effects of the plasma.

Jacob Brock
Eckerd College
T-4
Mentor: David Montoya

Presentation Title: Time Dependant Electron-Positron Pair Population in High-Energy Plasmas

Presentation Abstract: The electron-positron density in a plasma causes Compton scattering, increasing the plasma's opacity. In this project I am examining the electronpositron content of a plasma as determined by the initial electron content and the rates of creation and destruction of electron-positron pairs through the pair creation process and its inverse. In certain laboratory experiments not enough time passes for the equilibrium state to occur, so we need to know the time dependence of the process. Although the equilibrium electron-positron population of plasma is well known, the time dependant population has not been described as thoroughly. In this project I will set up the rate equations for the creation and destruction of these particle pairs and numerically integrate them to obtain the time dependence for the electron-positron population in the plasma. As the temperature of the plasma increases we see that the population of electrons-positrons increases greatly. As time permits, I may also examine how the presence of these additional particles can lead to cooling of the plasma by the Compton scattering and Bremsstrahlung processes. Finally, I will look at the time scales of various laboratory and astrophysical processes to see where this effect will be important.

Emily Chouinard
Michigan State University
T-6
Mentor: Siming Liu

Presentaiton Title: Modeling Electron Distributions and Radiation Spectra Produced in Gamma Ray Bursts

Presentation Abstract: Gamma Ray Bursts (GRBs) have become one of the greatest astrophysical phenomena during the past few decades. Their detection was quite accidental, and scientists have continuously studied them to unravel their mystifying nature. An aspect of GRBs that has become of great interest is the process of electron acceleration and the radiative processes responsible for most of the observed emission. These processes are critical for us to uncovering the underlying dynamical processes producing the GRBs. A code was developed to model the evolution of the electron distribution function under the influence of a turbulent magnetic field, which can be produced during the energy release of GRBs. This turbulent magnetic field can not only accelerate electrons to very high energies at the site of very efficient energy conversion, but also cool the electrons through the radiative processes in a more extended region, where most of the observed gamma-rays are presumably produced. There are three basic processes involved, namely the acceleration of electrons by turbulence, the escape of electrons from the acceleration site into a cooling region, the cooling of electrons through radiation. The electron distribution can be described by three basic parameters: the injection energy, the ratio of the acceleration to escape times delta, and the lifetime of the cooling region. Observational data can be compared with the model predicted synchrotron self-Comptonization spectrum to constrain the magnetic field, electron density, and the size of the emitting region.

Ian Faust
University of Michigan
P-24
Mentor: Tom Intrator

Presentation Title: Shielded Active Integrators for use in Plamsa Magnetic Field Diagnostics

Presentation Abstract: The Field Reversed Experiment (FRX-L) at Los Alamos National Laboratory confines deuterium plasma in a compact toroidal shape known as a Field Reversed Configuration (FRC). The characterization of the plasma necessitates the analysis of its magnetic fields. Through the use of Faraday's induction law, an electrical signal from a "b-dot" probe must be integrated accurately to understand the strength and nature of the induced magnetic field. Integration of the signal is done precisely using an analog active integrator. It allows for substantial gains, automatic zeroing of the baseline integrated signal and no signal droop, reducing the error. Data accuracy is preserved through diligent shielding from electromagnetic interference. This was done by mounting the cards within a standard rack chassis isolated in a faraday cage-like arrangement. The design has been optimized to reduce cross-interference, ease repairs and reduce temperatures. The overall error and noise fluctuations are expected to be reduced significantly by many orders of magnitude. Magnetic signal analyses, which comprise the primary diagnostic for the FRC, require one to difference two integrated dB/dt signals. This differential integrator provides a simple way to do this electronically without manually zeroing out integrating signals. The increased precision will allow for better characterization of the plasma in the upcoming tests on FRX-L. Depending on the time scales and characteristics of future plasmas, adjustments to longer timescales and greater shielding will necessitate modification of the active integrator.

Samuel Fletcher
Princeton University
P-25
Mentor: Gerd Kunde

Presentation Title: Jet Measurements for QGP Experiments at CMS

Presentation Abstract: Since the 1980s, experimentalists have sought to create in heavy ion collisions a new form of matter called quark-gluon plasma (QGP), where the constituent quarks of highly energetic hadrons become deconfined amidst large quantities of gluons—a kind of hot, dense "soup" in which the boundaries separating hadrons are no longer clearly defined. Measurements of the QGP can serve not only as a test of nonperturbative aspects of quantum chromodynamics, but also illuminate the properties of the early universe, which is believed to have existed as a QGP in the first few microseconds after the Big Bang. The most recent definitive successes in this endeavor have been at the Relativistic Heavy Ion Collider at Brookhaven National Laboratory, where gold nuclei were smashed together. One of the signs experimenters looked for was "jet quenching," a phenomenon where one side of a hard scatter is attenuated by the QGP's strong color field. A difficulty of these experiments, however, was that this very jet quenching hinders a determination of the energy loss from each jet, preventing accurate measurements of some of the QGP's properties. Hence a new experiment is being prepared for the Compact Muon Solenoid at the Large Hadron Collider, whose construction is nearing completion at CERN. This experiment uses the dileptonic decay of Z0 particles to tag the jets electromagnetically—one unhindered by the QGP's strong color field—thereby allowing for a precise determination of the energy of each jet. In this presentation, I will discuss some of the physics of these jet measurements and the experimental methods used to separate the Z0 signal from the background of other leptonic decay products.

John Gamble
College of Wooster
T-4
Mentor: Fernando Cucchietti

Presentation Title: Simulating a Quantum Ising Model on a Quantum Computer

Presentation Abstract: Since complex quantum systems cannot be simulated efficiently on classical computers, the advantage of using quantum computing could be enormous for computational physics. We investigate the simulation of the quantum Ising chain on a liquid-phase nuclear magnetic resonance (NMR) based quantum computer, which uses crotonic acid. Labeling one singly-coupled spin site in the molecule, we investigate the site's decoherence rate, which provides information regarding the simulation of the Ising chain on the remaining non-labeled atoms. We next determine the most effective site for the singly-coupled spin, and we numerically study the performance of different specific instruction sets using actual data from an experimental NMR quantum computer. Finally, we provide realistic measurement predictions in expectation of experimental implementation.

Tiffany Hayes
University of New Mexico
T-4
Mentor: Hanna Makaruk

Presentation Title: Measurement of Plasma Temperature

Presentation Abstract: Plasmas are an abundant source in the universe. The Sun is mostly plasma, and so is the gas around a black hole. Understanding how plasma reacts under any condition is an important step to understanding other processes. My mentor HANNA MAKARUK, of P-22, and me, of T-4, spent the summer with plasma data. We worked on trying to estimate the temperature of plasma under extreme conditions. The experiment consists of creating plasma with a short pulse laser. The process occurs in a matter of picoseconds. It is much too fast to relay on usual spectrometers. A camera takes series of spectral images during the process, and then we attempt to read the temperature from the continuous part of the spectra using an image processing program in Mathematica. The talk will present the techniques used during the process, and the results that were found.

Richard Korzekwa
University of Illinois, Urbana-Champaign
T-16
Mentor: Anna Hayes

Presentation Title: Hohlraum Reactions as a NIF Diagnostic

Presentation Abstract: Inertial Confinement Fusion (ICF) is one of two primary methods for producing controlled nuclear fusion reactions. In modern ICF experiments, a capsule containing fuel, typically deuterium and tritium (D-T), is compressed using a pulse of energy. At the National Ignition Facility (NIF), experiments will attempt to achieve ignition using an indirect drive apparatus in which a D-T capsule is placed inside a high-Z hohlraum in order to produce x-rays. One of the primary concerns for ICF is mixing between capsule and fuel, for which there does not currently exist a diagnostic at NIF. With an understanding of the effects of mix on the shape of the neutron spectrum, we can use several different reactions expected to occur within the hohlraum along with radiochemistry to infer some aspects of the neutron spectrum and hence make measurements concerning the level of mix taking place within the capsule. In addition, we may be able to make similar measurements for temperature or the asymmetry in capsule compression.

Richard Kraus
University of Nevada, Reno
P-24
Mentor: Eric Loomis

Presentation Title: An Improved Design for Explosively Driven Flyer Plates

Presentation Abstract: Explosively driven flyer plates are an important tool used in many shock physics experiments. Using this technique, synchronization of the shock loading with the diagnostics is much simpler than that of a gas or powder gun technique because of the relatively well known detonation time and short flight path. Also, it is a relatively portable experiment, compared to a large pulsed laser system, or in other words, you can bring the experiment to the diagnostics. This is advantageous for diagnostics like proton radiography or neutron resonance spectroscopy (NRS) at
LANSCE, where the diagnostics are immobile and there is no high energy pulsed laser system in the immediate area. The previous design for an explosively driven flyer plate was made by Charles Forest et al. [1]; however, there is evidence, both experimental and computational, that the Forest Flyer system causes the flyer to be curved, introducing another dimension of complication. Swift [2] improved upon this design in changing the geometry of the high explosive casing such that the flyer plate is now flat and the shock induced in the target is essentially one-dimensional. In the current research, further modifications in the design of the experiment have been made so as to decrease tensile
stress and spall in the flyer, decrease the curvature of the front and rear surface of the flyer, and determine a correlation between mass of the high explosive and velocity of the flyer. Comparisons have also been made as to multi-point initiation of the high explosive versus use of a plane wave lens to initiate detonation in the main charge. This design work has improved the accuracy of difficult bulk temperature measurements and decreased the amount of high explosives necessary to perform an experiment.

References:

1) C. A. Forest, R. L. Rabie, L. Bennett, and J Vorthman, in Proceedings of the 11th International Detonation Symposium, Snowmass, Co, 30 August to 4 September 1998. 2) D. C. Swift, C. A. Forest, D. A. Clark, W. T. Buttler, M. Marr-Lyon, and P. Rightley, Review of Scientific Instruments 78, 063904 (2007).

Tony Li
Cornell University
T-4
Mentor: Justin Oelgoetz

Presentation Title: The L ALPHA Spectra of Fe Ions

Presentation Abstract: X-ray spectroscopy of highly charged ions is an important tool in the study of high-temperature plasmas, especially distant astrophysical plasmas. For example, in He-like ions, the relatively strong K ALPHA spectral complex--lines arising from electron transitions between the 1s2l and 1s^2 configurations--has been studied extensively and serves as an effective diagnostic of both temperature and density. Less attention has been directed toward the L ALPHA spectral complex of He-like and Li-like ions, which results from transitions between the configurations 1s3l and 1s2l, 1s^23l and 1s^22l, or the 1s2l3l and 1s2l2l' states. These L ALPHA lines have lower energies, and as such may be more easily resolved by current instruments than the brighter K ALPHA complex. As they arise from the same ionization stages as the K ALPHA complex, they could be used as alternative diagnostics, particularly for Fe and other heavier ions, since the K ALPHA features of such ions are unresolved by current X-ray satellites. Using the code ATOMIC developed at LANL, we simulate both steady-state and time-dependent iron plasmas, focusing primarily on the L ALPHA lines. The resulting spectra cleanly break into distinct regions of Li-like, He-like, and H-like spectral lines. We then analyze the temperature dependence of these lines, as well as potential spectral signatures of cooling or recombining plasma.

Andrew Mastbaum
Lehigh University, Bethlehem, PA
P-23
Mentor: Andrew Hime

Presentation Title: Simulation and Characterization of Components of a Dark Matter Detector

Presentation Abstract: It is now firmly established that the matter content of the Universe is largely comprised of an unknown and non-luminous form. Astronomical observations and particle theory place WIMPs (Weakly Interacting Massive Particles) among the foremost of dark matter particle candidates. LANL scientists are currently leading efforts to develop a novel tonne-scale dark matter detector, which will observe WIMPs through recoils in a cryogenic noble liquid scintillation medium. Full detector simulations, supported by experimental tests of detector components (photomultiplier tubes, data acquisition systems, etc.) are key to the success of this pro ject. An overview of this pro ject will be presented, and results of detector simulations and photomultiplier tube testing will be shown.

Karen Miller
Texas A&M University
X-4
Mentor: Jeff Favorite

Presentation Title: Neutron Multiplication in Subcritical Systems

Presentation Abstract: There are at least five definitions of "neutron multiplication" currently used to describe subcritical neutron-multiplying systems. Preliminary calculations have shown that these values can vary by an order of magnitude depending on the interrogating source or the geometry of the system. To confuse the matter, experimentalists and computational scientists use the same vocabulary for different quantities. It is not well understood how multiplication inferred from measured data corresponds to different computed quantities of multiplication (net, total, leakage, keffective, and alpha). The objective of this research is to clarify these issues and determine the most suitable method for quickly computing the multiplication of subcritical systems. To do this, computational models using MCNP and PARTISN are compared to simulated or, when possible, actual measurements of simple, spherical and cylindrical systems. The research has applications for nuclear safeguards as well as characterizing accelerator-driven systems.

Dennis V. Perepelitsa
Massachusetts Institute of Technology
P-23
Mentor: Steve Elliott

Presentation Title: High-energy neutron-induced transitions in natural lead

Presentation Abstract: Fast neutrons incident on an atomic lattice can excite the nucleus and lead to a γ-cascade down to the ground state. Such neutron interactions in lead, copper, germanium and other shielding and detector materials may contribute to background in proposed neutrinoless double-beta decay experiments. This new generation of experiments will require energy sensitivity on the atmospheric neutrino scale (50 meV). To detect the faint double-beta decay signature, processes that contribute to background must be understood over a large range of incident neutron energies. A measurement of the neutron-interaction cross section can improve Monte Carlo simulations of expected background events. Here, the neutron interactions in natural lead are investigated quantitatively. In the late fall of 2006, a high-energy neutron beam experiment was performed using a natural lead target at the Weapons Neutron Research Facility at the Los Alamos Neutron Science Center. From this data, the integral γ-ray production cross sections in natural lead are determined for several important transitions in $^{206,207,208}Pb$ from neutron energies of 200 MeV down to interaction threshold. An analysis of experimental uncertainty is conducted.

Paul Tobash
University of Delaware
MPA-10
Mentor: Eric Bauer

Presentation Title: Heavy Fermion Compounds: Understanding the Strong Electronic Correlations in f- Electron Systems

Presentation Abstract: Heavy-fermion (HF) systems, those intermetallic compounds with extremely large electronic specific heat coefficients up to 1000 times larger than in simple metals like copper, have been the subject of much interest over the past few decades ever since the discovery of $CeCu_2Si_2$ in Germany and UBe_{13} here at Los Alamos. Since then, there has been a rebirth of investigations of these Ce, Yb, and Ubased intermetallics to better understand the heavy fermion state. The ultimate fate of a heavy fermion material is governed by a delicate balance between two competing interactions: the RKKY interaction, which promotes magnetic order, and the Kondo effect, which suppresses magnetic order. This delicate balance leads to a particular pressure dependence of the ordering temperature that has been observed in many Ce compounds such as $CePd_2Si_2$ and $CeIn_3$. Often superconductivity is found near where the magnetic order is suppressed to zero temperature, or quantum critical point. The search for isostructural Yb-based compounds is currently underway, which can be considered the ($4f^{13}$) hole analog to Ce's single ($4f^1$) f-electron configuration, with the goal of better understanding this electron-hole analogy between Ce and Yb and, possibly, finding an Yb superconducting heavy-fermion compound that has been elusive thus far. Preliminary efforts suggest the YbM_2X_2 and YbM_5X_2 systems (where M = transition metal, X = group 13 or 14 element) are promising candidates for these studies. It has been shown that the flux growth method is one way through which these materials are prepared thereby leading to large single crystals in pure phase. In this talk, I will discuss our synthesis and characterization including x-ray diffraction, magnetization, electrical resistivity, and heat capacity of new Yb- and Ce-based heavy-fermion compounds.