

Los Alamos National Laboratory

**Student Recognition &
Appreciation Week**

75th Anniversary Student Symposium Project Descriptions

**July 31, August 1 and
August 2, 2018**

**J. Robert Oppenheimer
Research Library**

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PADCAP

Individual Posters/Presentations

Materials Science

Student(s): Stafford, Michael Alexander

Program: USG/Postbac

School: New Mexico Institute of Mining and Technology

PAD/Group: PADCAP/PSI-PRTO

Mentor: Schake, Bradley Scott, PSI-PRTO

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26438

Introduction of a Fourier-Transform Infrared Spectrometer and Ellipsometer into a Radiological Facility

Installation of a Brooker Fourier-Transform Infrared Spectrometer (FTIR) and Woollam M-2000 Ellipsometer at PF-4 establishes enduring materials characterization of material properties of plutonium and other actinides. These capabilities support execution of the stockpile stewardship program; the enduring mission of Los Alamos National Laboratory (LANL) to confirm the safety, security, reliability, and performance of the nation's nuclear weapons. These technologies are utilized throughout industry and academia and will provide auxiliary support to existing capabilities. However, installation of complex instrumentation in a radiological facility requires a high degree of planning, investment of time and money and commitment to ensure radiological operations are safe, secure and effective.

Other

Student(s): Carnes, Cory L

Program: USG/Postbac

School: University of New Mexico

PAD/Group: PADCAP/C-DO

Mentor: Wong, Amy Suwu, C-DO

Category: Other

Type: Individual Poster

LA-UR: LA-UR-18-24990

Transfer of Pyrohydrolysis and Ion Chromatography Capabilities from Chemistry and Metallurgy Research Facility to Plutonium Facility

This poster will describe the requirements and challenges to successfully transfer of the pyrohydrolysis- ion chromatography (Pyro-IC) capabilities from the Chemistry and Metallurgy and Research (CMR) Facility to the Plutonium Facility (PF-4). Pyro-IC are common analytical techniques for determination of chlorine, fluorine and sulfur concentrations in a wide range of samples. The instrument currently residing in the CMR facility is a split-system. Fluorine and chlorine in actinide materials are volatilized by pyrohydrolysis technique at about 1000 degrees Celsius in a furnace and are captured in a stream of moist gas in a glovebox. The absorbed solution is then analyzed by an ion-selected electrode or ion chromatography instrument in a different lab room. The new system that will be installed into PF-4 is a state of the art instrument where a furnace, absorption cell, and ion chromatography are in an integrated system with the auto sampler. This automated system will significantly improve the safety and efficiency. To install Pyro-IC in a retrofitted glovebox in PF-4, there are significant challenges including glovebox modification, operability, maintainability, and ergonomics. The success in the installation and startup of Pyro-IC capability is essential in supporting program missions

Group Posters/Presentations Computing

Student(s): Kolkena, Ashleigh Ann; Salazar, Kayla Veronica; Sena, Joseph Paul; Slone, Llewelyn Richard; Valdez, Julien Luis

Student Names	University/School	Program	PAD/Group	Mentor
Kolkena, Ashleigh Ann	Utah Valley University	USG/Postbac	PADOPS/NIE-ESS	Marshall, Nicholas Redman, NIE-ESS
Salazar, Kayla Veronica	Northern New Mexico College	USG/Postbac	PADCAP/SSO	Whitaker, David Daleth, SSO
Sena, Joseph Paul	New Mexico State University	USG/Postbac	PADOPS/XIT-CSS	Lavy, April Lynn, XIT-CSS
Slone, Llewelyn Richard	University of California Los Angeles	USG/Postbac	PADOPS/SAE-3	Mcconaha, Christopher Warren, SAE-3
Valdez, Julien Luis	University of New Mexico-Los Alamos	USG/Postbac	PADCAP/SSO	Rivera, Deb, SSO

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-26181

After The Click

We will be tracing the path of malware from the click on an email to its conclusion on a single host. We will be analyzing alerts, host logs, and network logs.

Other

Student(s): Anaya, Lauryn Anne; Baca, Marissa Terese; Bennett, William Ira; Collins, Adam Paul; Haagenstad, Julia Marie; Montoya, Ryan Nicholas; Ramirez, Maricella Crystal; Williams, Tamia

Student Names	University/School	Program	PAD/Group	Mentor
Anaya, Lauryn Anne	University of New Mexico,	USG/Postbac	PADCAP/ADPM	Wood, Yvonne Barbara, ADPM
Baca, Marissa Terese	University of New Mexico	USG/Postbac	PADCAP/PADCAP	Wood, Yvonne Barbara, ADPM
Bennett, William Ira	University of Virginia	USG/Postbac	PADCAP/MOF-SU	Richardson, Scottie Lee, PM8
Collins, Adam Paul	Worcester Polytechnic Institute	USG/Postbac	PADCAP/MPD-PO	Borovina, Karen Garner, MPD-PO
Haagenstad, Julia Marie	University of New Mexico,	USG/Postbac	PADCAP/UI-DO	Witt, Monica Rene, UI-DO
Montoya, Ryan Nicholas	New Mexico State University	USG/Postbac	PADCAP/PM6	McClard, Deborah E, PM10
Ramirez, Maricella Crystal	Worcester Polytechnic Institute	USG/Postbac	PADCAP/PADCAP	Clarkson, Lynne, PADCAP
Williams, Tamia	Pennsylvania State University	USG/Postbac	PADCAP/UI-DO	Waldvogel, Genna Grace, ES-UI

Category: Other

Type: Group Poster

LA-UR: LA-UR-18-25649

Smart Lab Renovation in TA-35-0213

Since 1983, the Target Fabrication Facility was considered a state of the art laboratory. While its building features have been maintained up to this date, the technology is no longer appropriate for modern laboratories. Most of the HVAC equipment has outlived its lifespan. In addition, the lab hoods are similarly obsolete and in need of replacement or upgrades. Based on the demand for assessment ventilation report from 2017, a need for new HVAC systems is requested for TA-35-0213 (Target Fab). The purpose of this project is to implement SMART Lab features in Target Fab that will decrease energy consumption by 50% or more. In order to achieve this criteria, four auxiliary fume hoods will be replaced and an extensive cost and quality analysis will be conducted on the remaining 37 fume hoods to determine whether they have to be removed, hibernated, or retrofitted.

PADGS

Individual Posters/Presentations Computing

Student(s): Harter, Adam Tyler

Program: GRA

School: Missouri University of Science And Technology

PAD/Group: PADGS/A-4

Mentor: Rawlings, Chris, A-4

Category: Computing

Type: Individual Poster

LA-UR: LA-UR-18-25959

The Automated Design of Heuristics for the Traveling Thief Problem

Many real world problems require solving multiple computationally difficult, interconnected subproblems. The traveling thief problem (TTP), a combination of two well-studied problems, knapsack and traveling salesman, has recently been studied as a benchmark for difficult, interconnected problems. As a benchmark, the results for individual instances are not important, but heuristics that perform well could be translated for use in real-world problems. Despite the interconnected nature of the two subproblems, most current approaches to TTP solve the two parts separately. This work investigates the use of heuristic search techniques to automate the design of algorithms to find high quality solutions to families of TTP instances.

Student(s): Hollis, Andrew Nathan

Program: USG/Postbac

School: University of New Mexico

PAD/Group: PADGS/A-2

Mentor: Tompkins, George, A-2

Category: Computing

Type: Individual Poster

LA-UR: LA-UR-18-25533

Sensitivity Analysis for Netica® using the R Statistical Programming Language

One of the principle techniques used to evaluate Bayesian network models is sensitivity analysis. There are two types of sensitivity analysis: sensitivity to findings and sensitivity to parameters. Sensitivity to findings determines which nodes in the network, if their values were observed, would have the most influence on the distribution of some target node of interest in the network. Sensitivity to parameters determines which network parameters (i.e. conditional probability values), if varied, would cause the most variation in the distribution of some node of interest. The commercial Bayesian network software, Netica®, is equipped with sensitivity analysis for determining sensitivity to findings, but has no functionality for determining sensitivity to changes in parameters. We were able to use RNetica, a package for use with the R statistical programming language that allows R users to interact with the Netica® API, to create R functions that determine sensitivity to changes in parameters in Bayesian networks produced with Netica®. This additional analysis capability can help evaluate the stability of a model and identify a subset of parameters that warrant increased effort for their estimation.

Earth & Space Sciences

Student(s): Chakraborty, Shibaji

Program: GRA

School: Virginia Tech

PAD/Group: PADGS/ISR-1

Mentor: Morley, Steven Karl, ISR-1

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26196

Quantify Uncertainty in Probabilistic Kp Forecasting Models

Presentation Abstract: Space weather impacts various facets of our everyday life, from GPS navigation service accuracy to radiation dose on transpolar flights. Space weather effects at Earth are driven by a wide range of solar and solar wind phenomenologies. Geomagnetic storms, whose intensity are often described by a geomagnetic index (K_p), are a space weather phenomenon whose consequences can cost billions of dollars. Hence forecasting space weather is a major challenge addressing the security of modern technology. Current operational forecasts of geomagnetic indices use empirically-derived coupling functions or computationally expensive physics models to forecast short-term K_p , and neural networks for 3-to-12 hour ahead prediction. None of these methods provide error / uncertainty estimation associated with their forecast. For higher values of K_p the accuracy of current methods reduces and the models in use are unable to quantify the uncertainty associated with the prediction. This work aims to provide a K_p forecast for 3-to-24 hours with uncertainty bounds associated with each prediction. We will explore both parametric and non-parametric techniques to provide a probabilistic K_p forecast and quantify the uncertainty. Key factors in obtaining a good prediction include appropriate choices of model and training data. We used solar wind parameters to predict K_p . Using transformed solar wind parameters, historical K_p values and different transfer functions can increase the accuracy of the models. Our candidate models mainly use dynamic training sets to produce forecasts. In accordance with this we used variable training windows to find the best fitted model, providing insights about the solar wind parameters and solar cycle and how they affect the coupling to the geospace environment.

Student(s): Comellas, Jade Marie

Program: USG/Postbac

School: University of New Mexico

PAD/Group: PADGS/XIT-ISS

Mentor: Winter, Lisa Marie, ISR-1

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26356

Studying the Probability of Super Flares in Solar-Analog Stars to Predict Space Weather

Although our scientific understanding of space weather has dramatically increased over the last century, our technology is still very vulnerable to large solar flares and coronal mass ejections. In 1859, a major solar flare hit the Earth, greatly damaging telegraph systems and causing fires. However, because the technology at the time was not very sophisticated, the effects were not nearly as catastrophic as they would be if this were to happen today. Due to the current reliance on advanced technology for communication, transportation, and electricity, a geomagnetic storm of the same magnitude would cause devastating and expensive effects globally. Power grids, pipelines, and satellites would be destroyed. It has become a global safety obligation for space scientists to find ways to forecast these extreme space weather events. By studying stars that are similar to the Sun (solar-analog stars), we can better predict and understand solar flares. It has been found that some solar-analog stars not only have flares and coronal mass ejections but also super-flares, flares that are 100-1000 times greater in magnitude than the ones we have measured from the sun. By using data in SKYDOT's Northern Sky Variability Survey, a database that holds information from LANL's RAPTOR telescopes, we studied the changes in magnitude over time of known solar-analog stars to determine if any super-flare events have occurred. We identified the solar-analog stars by accessing an image of the area surrounding the star in the astronomical database SIMBAD and comparing it to a plot of the star's location from data in SKYDOT. Once a super flare is identified, this information is used to determine the probability of the Sun producing super flares of such magnitude.

Student(s): Czarnecki, Sean Michael

Program: UGS/Postbac

School: Arizona State University

PAD/Group: PADGS/ISR-2

Mentor: Gasda, Patrick J, ISR-2

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-25749

Detection of Subsurface High Silica Features on Mars Using Neutron Spectroscopy

In 2015, the ChemCam instrument on the NASA Curiosity rover observed significant silica enrichments in a lacustrine mudstone and an overlying aeolian sandstone on the lower slopes of Mt Sharp, the 5 km tall central peak of sedimentary rock in Gale crater. In this area, the Dynamic Albedo of Neutrons (DAN) instrument, a neutron spectrometer with a pulsed neutron generator and thermal and epithermal neutron detectors, observed elevated hydrogen abundances. DAN is sensitive to neutron scattering elements like hydrogen, and to neutron absorbers like iron and chlorine. The high silica, and correspondingly low iron, identified by ChemCam, combined with hydrogen enrichment, make these features observable in the subsurface by DAN. These anomalous elemental abundances prompted mineralogical analysis of the high silica material, which revealed the presence of tridymite, a high-temperature and low-pressure silica phase, and significant amorphous opaline silica, both of which suggest this feature originated as a volcanic deposit which was later altered by groundwater. Groundwater alteration is further supported by observations of high silica fracture 'halos' that cross-cut bedding and in some locations cross-cut the mudstone/sandstone contact. We compare DAN data to geochemical models created using the Monte Carlo N-Particle (MCNP) transport code developed at Los Alamos. This modeling constrains the water content of the unaltered bedrock, which is then used in more complex multiple layer subsurface models containing regions of both unaltered bedrock and high silica material. Using simulations with various geochemical compositions and high silica feature orientations and depths, we determine the subsurface geometry which best fits the DAN data from this area. Understanding the origin of these features can help us reconstruct aspects of Gale crater's geologic history, such as the duration, extent, and nature of groundwater activity.

Student(s): Sarrao, Joseph Hans

Program: High School

School: Los Alamos High School

PAD/Group: PADGS/ISR-2

Mentor: Wiens, Roger Craig, ISR-2

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26008

Characterization of the SuperCam Instrument for the Next Mars Rover

The SuperCam instrument is being built by LANL to provide remote sensing from NASA's next Mars Rover that is to launch in 2020. The Mars 2020 Rover will explore a new area of Mars and will collect samples for future return to Earth. SuperCam is patterned after LANL's ChemCam instrument that has been collecting chemical data on Mars for the last 6 years. Like ChemCam, SuperCam will use laser-induced breakdown spectroscopy (LIBS) to give the composition of rocks up to 7m from the rover. In the LIBS technique, powerful laser pulses focused on a target create brief plasmas that provide atomic emission spectra of the elements present. Additionally, SuperCam will study mineral compositions using remote Raman spectroscopy and infrared reflectance spectroscopy. SuperCam will also take close up images and record sounds on Mars. The team at LANL is checking the performance of an engineering prototype as we build the flight model. We are testing parameters to optimize the signal-to-noise. One such parameter is the exposure duration needed to capture LIBS plasmas. The longest feature of interest is a molecular calcium fluoride emission around 604nm. We are testing for its duration. Other parameters will be checked as part of the process of optimizing the instrument before it goes to Mars.

Student(s): West, Stephen Thomas

Program: GRA

School: Arizona State University

PAD/Group: PADGS/ISR-1

Mentor: Mesick, Katherine Elizabeth, ISR-1

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26076

Readout Electronics and Data Processing for Planetary Nuclear Spectrometers

Instruments sensitive to gamma ray and/or neutron radiation have been used since the Apollo 15 mission in 1971 to study the composition of planetary surfaces. Galactic cosmic rays (high energy protons) incident on the surface create fast neutrons through spallation. Subsequent interactions (capture, scattering) between these neutrons and the surface materials moderate the neutrons and produce a spectrum of characteristic elemental gamma rays. Additional gamma rays are produced through decay of radioactive isotopes. This project addresses two challenges for neutron and gamma ray instruments, namely: reducing size, weight, and power (SWaP) and developing data processing techniques to improve the spatial resolution of existing and anticipated future orbital datasets. Conventionally, separate detectors are used to measure both gamma rays and neutrons. CLYC (Cs₂LiYCl₆:Ce³⁺), a scintillator in the elpasolite family, is a promising detector material sensitive to both neutron and gamma ray radiation in which each interaction type has a characteristic pulse shape. Readout of scintillators is typically accomplished with photo-multiplier tubes (PMTs) however, silicon photo-multipliers (SiPMs) potentially offer a lower SWaP solution. We investigate the performance of an array of SiPMs coupled to a large (5cm x 5cm) CLYC crystal to mature the optimal read-out circuit design as well as data processing parameters. In addition to hardware maturation, this project studies spatial deconvolution algorithms for orbital neutron spectroscopy data. Uncollimated orbital neutron detectors have a field of view roughly equivalent to 1.5h, where h is the altitude above the surface. The Mars Odyssey Neutron Spectrometer (MONS) has acquired fast, epithermal, and thermal neutron counting rates from a ~400 km polar Mars orbit since 2002. Improving on the inherent ~550 km MONS spatial resolution requires deconvolving the neutron signal from instrument-induced smearing. We develop new algorithms to reconstruct MONS data at finer spatial scales in order to better resolve surface compositional variations.

Engineering

Student(s): Cox, Elaine M

Program: USG/Postbac

School: Duke University

PAD/Group: PADGS/ISR-4

Mentor: Merl, Robert Bernard, ISR-4

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25640

Extracting a Write Enable Signal from an MDIO Packet

The physical layer (PHY) to media Access Controller (MAC) interface is an integral part of an Ethernet connection. These connections allow for circuit boards to communicate faster with less excess weight. Field Programmable Gate Arrays (FPGAs) can help create this interface, but can be limited by the cores they contain. While the PHY-MAC interface traditionally communicates through management data input output (MDIO), some cores anticipate separate input and output signals, as well as an output enable signal. This project looked to develop VHDL code for the FPGA to extract the output enable signal from the MDIO packet. This allows for the use of these cores to better suit board communication in space flight use, among others.

Student(s): Elder, Jessica Marie

Program: USG/Postbac

School: Worcester Polytechnic Institute

PAD/Group: PADGS/NEN-2

Mentor: Grove, Travis Justin, NEN-2

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26496

Investigating Fit Accuracy of Startup Counter Data to Predict Uncertainties in Period and Reactivity Measurements

Neutron detection systems are used to measure neutron leakage from outside of assemblies and can be used to determine how the neutron population in the assembly is changing with respect to time. If a nuclear assembly is supercritical, the neutron population (as well as the neutron leakage) will exponentially increase as a function of time, with the reactor period being the time it takes for the neutron population to increase by a factor of Euler's number. The reactivity of the assembly is related to the reactor period through the Inhour equation. Both the reactor period as well as the reactivity of an assembly are important in studies of nuclear assemblies. One type of neutron detection system used at the National Criticality Experiments Research Center (NCERC) is the Startup Counter, which is a Helium-3 (He-3) based neutron detection system. Neutrons are absorbed by the He-3 gas, which releases charged particles that can be detected in a proportional counter. Each neutron detection creates an electronic pulse in the detector electronics, which can be counted and recorded. These detector pulses are recorded using a LabVIEW program, which can then plot the recorded data and perform basic curve-fitting to selected data. This basic curve-fitting is used to find the reactor period and reactivity of a supercritical assembly at NCERC. However, the LabVIEW curve-fitting results do not give any indication of the errors associated with the reactor period and reactivity measurements. This research aims to determine the expected errors in period measurements from theoretical supercritical measurements. Since counts of spontaneous fissions are assumed to follow a Poisson distribution over large time intervals, applying this distribution to a set of exponentially increasing data points can be used to model theoretical data from measuring a supercritical assembly. This model was implemented into R Programming, and fit parameters – including period – were obtained. A Monte Carlo approach was then used to find the distribution of period measurements, and therefore the highest errors that are likely to occur from the LabVIEW estimation. It was found that increasing the overall number of counts decreases the expected error. Multiple factors can change the number of counts, and therefore the expected error, including the source type and the time frame of measurement.

Student(s): Fresquez, Reuben Anthony

Program: USG/Postbac

School: University of New Mexico

PAD/Group: PADGS/ISR-3

Mentor: Michel, John M, ISR-3

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26209

Mars 2020 SuperCam Computerized Data Analysis

The Mars 2020 SuperCam instrument utilizes a camera, lasers, and spectrometers to collect and examine data from rocks and soils on Mars. The SuperCam instrument produces large data sets that can be difficult to interpret. Using sorting, data analysis, and comparator algorithms we can provide readable data for others to interpret and use while studying Mars. Spectral data is generated when light is split into its spectral components using optical gratings and then focused onto a charge-coupled device containing up to 3 spectral regions, each with 2148 channels. The data from the collected spectra is stored in an array for each channel within a region. As a data reduction technique, statistical analysis can be performed, and the arrays must be sorted quickly in the onboard flight software. I investigated sorting algorithms choosing the algorithm with the least overhead and time consumption, and then implemented it in the flight software. In addition, as part of the instrument's software development and testing, there is a need to regularly execute scripts of SuperCam commands and verify the resulting binary data. Without an automated process, data analysis can become costly and time consuming. Much of the telemetry data contains time stamps, voltage, and temperature data that may change from test to test. However, much of the data needs to be checked for consistency. I wrote an application to parse and compare the telemetry data to known good data in an extensible way such that the same technique can be applied to other command scripts.

Student(s): Fritz, Dominik Arthur

Program: USG/Postbac

School: Rensselaer Polytechnic Institute

PAD/Group: PADGS/NEN-2

Mentor: Cutler, Theresa Elizabeth, NEN-2

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26161

Genetic Algorithm Based Experimental Design for Uranium Cross Section Validation

Nuclear data is vital to the safe design of any nuclear system, whether it's a nuclear reactor or a radiation detector. Due to the strong dependence of modeling and simulation on the accuracy of the underlying differential nuclear data, it is paramount that the neutron cross section data used in various codes is properly validated and verified. Historically, the use of critical experiments, or zero power reactors, have been the primary method to validate neutron cross section performance in radiation transport codes. Critical experiments are designed to have their neutron multiplication factor very dependent on, or sensitive to, the cross sections of interest such that a small deviation in the cross section value will result in a large change in the multiplication of the system. Coupling this sensitive behavior with various critical configurations can help validate cross sections. Although many experiments have been performed to characterize the U-235 neutron cross sections in the intermediate energy region, the 2.25 keV – 25 keV energy region still remains unresolved. The Unresolved Resonance Region (URR) of the U-235 fission cross section continues to need validation in order to improve safety analysis of all uranium based systems. An integral experiment design involving the use of a vertical assembly machine, a copper reflector and high enriched uranium metal with interstitial material has been proposed to further validate these cross sections. Interstitial materials of interest have been selected from previous work involving a physics-based approach. Utilizing these interstitial materials in simulations with MCNP6 and ENDF libraries, a unique critical experiment will be designed and optimized by a genetic algorithm, maximizing relative sensitivity to the fission cross sections in the URR.

Student(s): Giha, Nathan Patrick

Program: USG/Postbac

School: University of Michigan

PAD/Group: PADGS/NEN-1

Mentor: Ruch, Marc Lavi, NEN-1

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26289

Resolving Position of Fission Sources in He3 Well Counters w/ List-Mode Analysis

The ^3He thermal neutron coincidence counter is used in the field of nuclear safeguards to measure the mass of special nuclear material (SNM) in a sample. Coincidence counters measure the spontaneous fission neutron signature of SNM to determine the mass. The International Atomic Energy Agency (IAEA) has used neutron coincidence counters since the 1970s to verify mass declarations of SNM in a container. The neutron coincidence counter is designed to be insensitive to the location of the fission source within its well. This is often a desirable trait, as the detector operator need not concern themselves with measurement geometry. However, the counter consequently is susceptible to spoofing scenarios in which there are two spatially separated sources when only one was declared. Thus, the instrument would ideally retain its insensitivity to fission source location for total mass measurements, while also detecting such a spoofing scenario. A list-mode post-processing technique was developed to resolve the position of a fission source within a ^3He neutron well coincidence counter. The technique operates on the principle of analyzing the pulse trains of specific ^3He tubes. This poster describes the underlying principles of this technique

Student(s): Gnawali, Krishna Prasad

Program: GRA

School: Southern Illinois University Carbondale

PAD/Group: PADGS/ISR-3

Mentor: Quinn, Heather Marie, ISR-3

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25600

Pulsed Laser Testing of Single-Event Transients in a LM124 Operational Amplifier

All modern electronic components are affected by radiation that occurs in space and the Earth's atmosphere. Circuits that are exposed to radiation may have faulty behavior and cause system failure. The impinging radiation particles degrade the switching capabilities of transistor and introduce single-event effects (SEEs) which are instantaneous temporary errors. Shrinking feature size makes transistors more vulnerable to SEE. Therefore, it is of high importance to test the circuit for radiation hardness. Typical test procedure involve the use of particle accelerators. This poster demonstrates the impact of radiation on the LM124 operational amplifier using a pulsed laser and the correlation of previously published results obtained at particle accelerators.

Student(s): Hagopian, Victoria Elizabeth

Program: GRA

School: Penn State University

PAD/Group: PADGS/NEN-2

Mentor: Goda, Joetta Marie, NEN-2

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26329

Updating the Godiva-IV Benchmark

Updates were made to the Godiva-IV benchmark model to account for updated spindle and glory-hole dimensions and the discovery of a shim found during disassembly. An updated version of the Top Hat, an aluminum contamination shield, was added to the model as well to study the effects this removable component had on the value of k_{eff} for the system. With the additions complete, a comparison between the ENDF/B-VII.1 and ENDF/B-VIII.0 cross-section libraries was performed using MCNP[®] [1]. Using the newer ENDF/B-VIII.0 libraries resulted in values of k_{eff} that were much closer to the experimental values for Godiva-IV, 0.99847 ± 0.00032 and 0.99646 ± 0.00028 for the cases with and without the Top Hat, respectively. Further improvements were made to the model to improve the user friendliness in adjustment of the moveable components in the assembly. Users can now specify the location of the burst rod, both control rods, and the safety block. More detail will continue to be added to the model such that it mimics the previously used “detailed models.” Once development is complete, sensitivity testing will be performed to demonstrate how unknowns in the experiment compare to the Monte Carlo model as was performed in the existing benchmark, HEU-FAST-MET-086.

Student(s): Hua, Michael Yeungjun

Program: GRA

School: University of Michigan

PAD/Group: PADGS/NEN-2

Mentor: Hutchinson, Jesson D, NEN-2

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26158

2-Exponential Behavior and Degree of Separation Invariance in Rossi-alpha Histograms

The subcritical reactivity of a neutron multiplying system is often of interest in nuclear nonproliferation and criticality safety applications. The subcritical reactivity can be inferred from the prompt neutron decay constant, α . The Rossi- α method is a subcritical analysis technique that utilizes neutron time-correlation characteristics to determine α . In the analysis, a histogram of the times between a neutron detection and following detections is produced. α is determined from a fit of this histogram. Traditionally, a single-exponential fit is used. In this poster, a double-exponential fit is developed from first principles which ultimately allows for analytic uncertainty approximation. The double-exponential is more appropriate for reflected/moderated systems. The system reflector/slowing-down time and α are calculated and the respective uncertainties are estimated. In this work, a 4.5 kg sphere of plutonium called the BeRP ball (Beryllium-Reflected Plutonium) was measured with the NoMAD He-3 gas proportional counter detection system. The measurement was simulated with MCNPX-PoliMi, and the simulated data matches the measured data well. A neutron that initiates a fission chain is said to come from generation 0. Neutrons born from a fission induced by a generation j neutron are said to be generation $j+1$ neutrons. MCNPX-PoliMi allows users to easily track a neutron's generation. For two neutrons originating from the same fission chain, δ is defined as the degree of separation. For example, neutrons of generation numbers $j+n$ and j in the same fission chain have a δ equal to n . In this poster, the simulated data shows that the calculated α -value is independent of δ .

Student(s): Mullin, Elinor Rainbow Ruth

Program: USG/Postbac

School: Fort Lewis College

PAD/Group: PADGS/ISR-1

Mentor: Nowicki, Suzanne Florence, ISR-1

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25977

Pre-deployment Characterization of Large Fast Neutron Detectors for High Performance Computing Fault Characterization

Los Alamos National Laboratory (LANL) provides world-class high performance computing (HPC) capabilities, which is a vital resource for a wide range of science. It is important that these systems are reliable and produce results that scientists can depend on. Computers have long been known to be impacted by neutrons. Supercomputers can experience faults in their microprocessors in the form of data corruptions and crashes caused by the interaction of neutrons. These events are known as single event upsets (SEU). The understanding of the neutron environment in the Strategic Computing Complex (SCC) at LANL, where the supercomputers are located, is critical for understanding the risks of neutrons to the supercomputing hardware. In collaboration with the Space Science and Applications group (ISR-1) at LANL, the HPC Design Group (HPC-DES) purchased several plastic and liquid scintillator neutron detectors to be deployed in the SCC to monitor the cosmic neutron intensity over time. This study investigates and compares the pulse shape discrimination (PSD) capabilities of two of the neutron detectors that will be deployed in the SCC; one plastic Eljen (EJ)-299-33A detector and one liquid EJ-309 detector, both 12.7 centimeters in diameter and length. At an energy window of 0.8 to 1.0 MeVee, the plastic scintillator detector has a figure of merit (FoM) value of 1.098. With this characterization and deployment of the detectors, a more complete understanding of the cosmic neutron intensity in the SCC is possible and the vital work at the HPC will be more reliable.

Student(s): Mummah, Kathryn Ann

Program: GRA

School: University of Wisconsin-Madison

PAD/Group: PADGS/NEN-2

Mentor: Bahran, Rian Mustafa, NEN-2

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26424

Simulation of the Nuclear Fuel Cycle for International Safeguards

As part of a comprehensive safeguards evaluation, Acquisition Path Analysis (APA) of a State provides a method to “analyze the plausible paths by which, from a technical point of view, nuclear material suitable for use in a nuclear weapon or other nuclear explosive device could be acquired” APA is part of an effort by the International Atomic Energy Agency (IAEA) to maximize the efficiency and effectiveness of international safeguards by considering each State as a whole and not just a collection of individual facilities. Nuclear fuel cycle simulators (FCS) codes are fundamentally tools to track material as it undergoes chemical and nuclear changes and moves between facilities in a nuclear fuel cycle. The ability to model facilities at high fidelity creates the opportunity to study the material throughput in an individual facility, for a potential acquisition path, or for a full set of nuclear facilities mimicking a State. This throughput tracking can also be coupled with the ability to study dynamic scenarios where facilities may be opening, retiring, or ramping up (down) in production. The use of FCS tools has the ability to add in-depth modeling capability to APA and inform the continued effort to increase the efficiency and effectiveness of international safeguards.

Student(s): Naranjo, Mario Reyes

Program: GRA

School: University of New Mexico

PAD/Group: PADGS/NEN-5

Mentor: Kim, Jun, NEN-5

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25290

Nek5000 Capabilities in Thermal Fluid Flow Applications

Created at Argonne National Laboratory's Mathematics and Computer Science Research Division, Nek5000 is an open-source computational fluid dynamics (CFD) code created for simulating unsteady incompressible flow with thermal and passive scalar transport. Several open-source CFD code are available, each most commonly created with specific an application in mind. The presence and reliability of project support and development community is another consideration when choosing and open-source CFD code. For our purposes, studying the heat transfer of a heating element immersed in water, using a code developed for incompressible flow and supported by another national laboratory appears to meet both our criterion. The process of running a simulation in Nek5000 consists of three primary steps: pre-processing, solving, and post-processing. Pre-processing consists of creating a mesh, defining initial and boundary conditions, and other parameters. The solver is a spectral element time-stepping code written in C and Fortran 77, which supports either Open MPI or Intel's NX message passing libraries. For post-processing a script is run, creating a file, which is then visualized using VisIt or ParaView. Nek5000 comes with many example cases providing both references and templates to aid in creating new simulations. I will begin with classical examples of CFD problems, working towards more complex and topic specific cases. The first case is of two-dimensional pipe flow with uniform heat flux at the wall. The next is of two dimensional natural circulation in a rectangular computational domain. Continuing on to create and/or modify cases to increase my understanding of Nek5000's capabilities and how they can be used to best meet my group's objectives. Throughout this process I will also learn of Nek5000's user support network as I create new and varying test cases. Nek5000 is continually being developed and supported as it gains acceptance and grows within the CFD community.

Student(s): Youmans, Amanda Elizabeth

Program: GRA

School: Rensselaer Polytechnic Institute

PAD/Group: PADGS/NEN-1

Mentor: Trahan, Alexis Chanel, NEN-1

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25739

Comparison of DDSI experimental and simulated results

The Nuclear Engineering and Nonproliferation Safeguards Science and Technology (NEN-1) group develops detector systems for the International Atomic Energy Agency to use for safeguarding special nuclear material. The Differential Die-away Self-Interrogation (DDSI) instrument was designed to characterize spent fuel assemblies. DDSI uses helium-3 detectors to count time-correlated neutrons to determine the fissile content of an assembly. The neutron counts are recorded for each detector as a function of time, i.e. in list mode. By using the list mode data acquisition method, advanced analysis techniques such as Rossi-Alpha Distributions (RAD) can be used to gain more information about the fuel assemblies. The neutron singles rate, doubles rate, and RAD are used to verify assembly parameters including multiplication, burnup, initial enrichment, and cooling time. This system was tested in the Clab interim fuel storage facility in Sweden using a set of 50 well-characterized spent fuel assemblies collectively called the SKB50. These fuel assemblies were modeled in MCNP and integrated with a model of DDSI to generate simulated neutron detection data. Detection results can be generated for each bank of detectors as well as for each individual detector channel. The simulation can be used to determine a singles rate, doubles rate, and RAD which can then be compared to experimental data collected in Sweden to validate the models. After the model is validated, it can be used to quantify sensitivity of the neutron detection rate to assembly positioning, as well as accuracy of the SKB50 fuel assembly models. Inaccuracies in the fuel assembly models are expected because of the challenges in modeling spent nuclear fuel, namely inaccurate or incomplete nuclear data. Finally, the simulated BWR measurement results can be used to quantify and correct for axial heterogeneities which affect the assembly characterization. In this way, MNCP simulations are used to support the experiments.

Mathematics

Student(s): Sanna Passino, Francesco

Program: GRA

School: Imperial College London

PAD/Group: PADGS/A-4

Mentor: Turcotte, Melissa, A-4

Category: Mathematics

Type: Individual Poster

LA-UR: LA-UR-18-26428

Latent feature models for network link prediction with labelled nodes

In cyber networks, relationships between entities, such as users interacting with computers, or system libraries and the corresponding processes that use them can provide key insights into adversary behaviour. Many cyber attack behaviours create new links between such entities - previously unobserved relationships. A probabilistic latent feature model is presented to predict the formation of new edges between entities in computer networks enabling anomaly scores to be assigned to new link formations over time. In particular, the Poisson matrix factorization model is extended to include known covariates about each entity or node. Results show that the including known covariates about each entity can improve predictive performance enhancing anomaly detection capabilities.

Physics

Student(s): Lucero, Reyes Kerry

Program: USG/Postbac

School: Coe College

PAD/Group: PADGS/ISR-3

Mentor: Dreesen, Wendi M, ISR-3

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26162

Designing and implementing a helical feed antenna

The goal of this summer project was to design and test a new feed antenna for the Los Alamos Portable Pulser(LAPP). The project was intended to provide an introduction to working with radio frequency. It was also intended to test alternate feed antenna options for the LAPP. The LAPP is used to test space based VHF sensors. Pulsed power is currently sent through a bow-tie feed antenna to a parabolic dish before being reflected into space. Originally, a helical antenna was used to feed the dish but was replaced with the current bow-tie design. A helical design was recently desired due to its better performance in the high band (~150MHz) as well as emitting circularly polarized radiation. The trade-off is worse performance in the low band (~30MHz). John Kraus did extensive research into helical antennas and documented it in his book Antennas. Based on his research, I designed a helix with a center frequency of 100MHz. Jeremiah Rushton provided simulations of my design. His data show that the gain in the lower bands remains satisfactory with increased performance in the high band as compared to the bow-tie feed. With help from Bobby Quintana, a dielectric PVC endoskeleton will be constructed to support the wound copper tubing. The preexisting ground plane will remain. Power is fed from a 130 Joule Marx bank to the antenna. Matching the antenna impedance to the Marx bank is difficult especially because the antenna's impedance changes as a function of frequency. Furthermore, traditional helices implement a gradual feed through the ground plane to help with impedance matching. Unfortunately, our Marx bank generates over a million volts, so a gradual taper creates real potential for arcing.

Student(s): Minard, Aaron Russell

Program: USG/Postbac

School: Greenville University

PAD/Group: PADGS/ISR-5

Mentor: Quintana, Bobby Arthur, ISR-5

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26349

Consideration of Pulse Power Options and Design Optimization

I work with a system requiring the emitting of a high powered VHF signal. We currently use a Marx bank for generating a pulse to create this signal. I'm researching several methods of generating pulse power for this and other applications. I am also researching methods for optimizing each method for higher reliability, cost and size reduction, and less power required if lower impedance is achieved.

PADOPS

Individual Posters/Presentations

Biosciences

Student(s): Curtis, Jessica Ryann

Program: GRA

School: Oregon State University

PAD/Group: PADOPS/RP-PROG

Mentor: Mann, Jenelle Elicia, RP-PROG

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26226

Comparison of Attila and MCNP Methods

Due to their complex nature, radiation shielding and dosimetry modeling are routinely performed using Monte Carlo methods such as Monte Carlo N-Particle Transport Code. While MCNP is known for its high accuracy, long run times due to optimization of variance reduction techniques as well as significant time spent by the user defining the problem domain provide challenges in evaluating new and existing designs efficiently. Attila advertises features which have the potential to reduce time and computational cost while maintaining accuracy, such as a deterministic solver and CAD integration. With direct CAD integration, Attila has the potential to provide quick manipulation of designs effectively reducing the time required to evaluate designs for compliance with worker dose regulations. Attila is of interest to the Radiological Engineering Program, as Radiological Engineers regularly analyze complex facilities and geometries. This project compares Attila against MCNP codes for simple source geometries as an initial evaluation of the accuracy and efficiency between the two codes.

Engineering

Student(s): Smith, Savanna Kalehua Easton

Program: USG/Postbac

School: The University of Texas at Austin

PAD/Group: PADOPS/UI-DO

Mentor: Waldvogel, Genna Grace, ES-UI

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25374

Feasibility Study of Non-Potable Water for Future Supercomputer Infrastructure

To support future generations of high performance computers, the Advanced Simulation and Computing Program has a mission need for 80MW of peak power and cooling. Currently, the super computers at the SCC are cooled mostly with Sanitary Effluent Recovery Facility (SERF) water. When SERF water is not available, potable water is used. The amount of water that the SCC needs nominally is around 45 Mega-Gallons/Year (MGY). The future super computer infrastructure (FSI) will need around 125 MGY nominally. The SERF reclaimed water production is approaching its limit. In order to avoid using 100% potable water for the FSI, the option of using non-potable reuse water from Los Alamos County was analyzed. The analysis conducted verified the volume of non-potable (NP) water available from LAC along with the cooling needs of the FSI. The two best locations for the FSI in terms of water infrastructure were determined as well as pipe sizing and interconnection points for each of these locations. The status of existing pipes, water storage, pumps, capacity, and location were analyzed. The quality of water needed for operation of the cooling was decided along with any additional treatment needs. A cost analysis was completed for the use of NP & potable water and their associated infrastructure.

Health & Safety

Student(s): Giddings, Antoine Duane

Program: USG/Postbac

School: ALCORN STATE UNIVERSITY

PAD/Group: PADOPS/RP-SVS

Mentor: Mclean, Thomas Donaldson, RP-SVS

Category: Health & Safety

Type: Individual Poster

LA-UR: LA-UR-18-26124

Type Testing of Selected Health Physics Instrumentation

This project involves the type testing of several recently acquired health physics instrumentation. Type testing is used to better understand the capabilities and limitations of instruments and they are required according to RP-SVS procedures. An environmental chamber (Thermotron 8200) has been used to study the response of selected instruments to a wide range of temperatures and humidities. The test protocols and acceptable instrument performance criteria follow those outlined in ANSI N42.17A. The instruments tested during this project included the RadEye PX rate meter with the Ludlum Model 43-32 probe, the RadEye GX rate meter with the Thermo Model HP-270 probe, and the RadEye SX rate meter with the Ludlum Model 43-93 probe.

Student(s): Linn, Jacqueline Ann

Program: USG/Postbac

School: Los Alamos High School

PAD/Group: PADOPS/OSH-OH

Mentor: Chan, Martha Kwan Yi, OSH-OH

Category: Health & Safety

Type: Individual Poster

LA-UR: LA-UR-18-25510

The Effects of Footwear Products on Worker's Comfort

A glovebox is a containment unit that protects the worker from the materials inside the box and vice versa. These gloveboxes generally sit on cement floors, which can cause problems for the workers when they stand to work for extended periods of time. There are approximately 400 workers performing glovebox work in PF-4. In effort to help the workers, the TA55's ergonomics team tested the ErgoMates® anti-fatigue matting overshoes stocked in the TA55 warehouse against MEGAComfort® PAM anti-fatigue insoles recommended at a VPP conference. 36 workers participated in this study. Participants were asked to wear their own normal footwear and each of the anti-fatigue products separately over a 3-day period. During the study, workers were asked to complete two surveys each day, indicating their discomfort and fatigue levels in the morning and at the end of the work day. The resulting data shows that while ErgoMates do not make a significant change in fatigue and discomfort levels when tested against normal footwear with no anti-fatigue products, the MEGAComfort PAM insoles did show a significant decrease in end-of-day worker fatigue level compared to not wearing any anti-fatigue products. Based on this study's results, it is recommended that MEGAComfort PAM insoles should be stocked.

Student(s): Preddie, Alaina Katelyn

Program: GRA

School: The Ohio State University

PAD/Group: PADOPS/OSH-OH

Mentor: Chan, Martha Kwan Yi, OSH-OH

Category: Health & Safety

Type: Individual Poster

LA-UR: LA-UR-18-25701

Glovebox Workers' Range of Motion in Three Gloveports

Gloveboxes are enclosed workstations used to protect workers, the environment, and/or the materials within the glovebox itself. Work in a glovebox is done through secured gloved openings called gloveports. Department of Energy laboratories, as well as facilities in other industries, utilize gloveports with different shapes and orientations. There is no documented data regarding worker preference or range of motion working in different gloveports. The aim of this study was to obtain data on worker range of motion limitations and preference in three gloveports: round, vertical oval, and 45° offset oval. 35 experienced glovebox workers performed two reach tasks in each gloveport type to assess range of motion limitations. Participants then rated the ease or difficulty to accomplish tasks in each port and selected their port preference. Results of this study showed a greater reach distance for the vertical oval gloveports compared to both the round and 45° offset oval gloveports. Participants rated the vertical oval gloveports significantly easier to work in than both the round and 45° offset oval gloveports. Additionally, participants selected the vertical oval gloveports as their preferred gloveport.

Student(s): Simpson, Chason Thomas

Program: USG/Postbac

School: Santa Fe Community College

PAD/Group: PADOPS/RP-SVS

Mentor: Moore, Murray E, RP-SVS

Category: Health & Safety

Type: Individual Poster

LA-UR: LA-UR-18-25021

Filter media in continuous and fixed air samplers for alpha emitting aerosols

The Los Alamos National Laboratory and the Pacific Northwest National Laboratory utilize various filter materials for different continuous air monitors and fixed air samplers. In a cooperative effort between the two institutions, (1) the flowrate per unit area per unit pressure, (2) the alpha spectrum resolution, (3) the radon progeny interference for plutonium alpha decay detection, (4) the radon progeny collection, and (5) the aerosol collection efficiency will be measured for seven different filter types. These filter types include glass fiber, mixed cellulose ester membrane, and polytetrafluoroethylene (e.g. Teflon®) membrane filter compositions. The five different metrics represent three major features that are typically considered in the use of filter media for the air sampling of airborne radioactive alpha emitting substances. These features (Hoover and Newton 1991) have been identified as (A) the amount of particle collection on the filter face, compared to burial of the particles within the matrix of the filter material (burial tends to degrade the measured alpha energy spectrum), (B) the aerosol particle collection efficiency will affect the measured value of sampled radioactive material, (C) the pressure drop for a given flowrate will depend on the filter composition and the active filter diameter. The five different metrics will be measured with a set of Canberra® Alpha Sentry™ continuous air monitors for the flowrate and alpha spectrum related quantities, and with TSI Inc® aerosol particle spectrometers for the aerosol collection efficiency values, over nanoparticle and micron-sized particle ranges.

Other

Student(s): Fellows, Samara Kia

Program: GRA

School: Jefferson University

PAD/Group: PADOPS/OSH-OH

Mentor: Splittstoesser, Riley, OSH-OH

Category: Other

Type: Individual Poster

LA-UR: LA-UR-18-26504

I'll Think of a Title for This Later: The Costs and Benefits of Procrastination

People delay tasks every day; whether it's completing a poster, starting a diet tomorrow, or making important decisions. The fact is that procrastination happens; different people do it for different reasons. The aim of this review is to determine the costs and benefits of procrastination and to see if it really is worth procrastinating. Databases such as ScienceDirect Journals, PsycINFO, and JSTOR: Arts and Science Collection were used to search for primary research. Procrastination can be marked by few short-term benefits and many long-term costs with the costs outweighing the benefits

Student(s): Sanchez, Jonathan Christian

Program: USG/Postbac

School: FT Lewis

PAD/Group: PADOPS/EPC-ES

Mentor: Montalvo, Maryrose L, EPC-ES

Category: Other

Type: Individual Poster

LA-UR: LA-UR-18-25970

Going Paperless at LANL

For companies everywhere, the digital age has taken over. "Going paperless," refers to the process of moving all documents, files, and records into a digital format. The process can be time, labor and cost intensive, all contingent on the magnitude of the organization's document retention needs and requirements. At Los Alamos National Laboratory, "paperless" alternatives began surfacing in concert with mission requirements and unexpected events such as the Cerro Grande Fire. The 2017 Environmental Management System (EMS) Audit presented LANL with an opportunity for improvement (OFI) to identify paperless capabilities institutionally available and raise awareness about their existence. The EMS opportunity for improvement is also an opportunity to learn about paperless initiatives in classified and unclassified environments that have standardized practices and implemented efficiencies at LANL.

Group Posters/Presentations Computing

Student(s): Duran, Valerie R; Quintana, Lauren Ann; Vargas, Alex

Student Names	University/School	Program	PAD/Group	Mentor
Duran, Valerie R	CSU	UGS/Postbac	PADOPS/XIT-CSS	Ortiz, Melissa, XIT-CSS
Quintana, Lauren Ann	UNM	UGS/Postbac	PADOPS/XIT-CSS	Ortiz, Melissa, XIT-CSS
Vargas, Alex	Northern New Mexico College	USG/Postbac	PADOPS/ISR-3	,

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-26457

Virtual Desktop Infrastructure Proof of Concept

A Virtual Desktop Infrastructure (VDI) proof of concept that utilizes industry leading technologies such as Cisco Unified Computing System (UCS), NetApp, VmWare Horizon, vCenter and eSXi as well as Red Hat Enterprise Linux (RHEL) with the goal to replace the Sun Ray thin client. This project focuses on implementing a back-end environment that consists of UCS blade servers connected to a NetApp via NFS, iSCSI and 40Gbps uplinks to provide computing resources for VmWare eSXi and Horizon. This highly available back-end environment consists of two eSXi hypervisors that are managed by a vCenter Virtual Machine (VM). In addition to a back-end environment, a front-facing user friendly environment must be setup as well, for both our users and our support teams.

Student(s): Kolkena, Ashleigh Ann; Salazar, Kayla Veronica; Sena, Joseph Paul; Slone, Llewelyn Richard; Valdez, Julien Luis

Student Names	University/School	Program	PAD/Group	Mentor
Kolkena, Ashleigh Ann	Utah Valley University	USG/Postbac	PADOPS/NIE-ESS	Marshall, Nicholas Redman, NIE-ESS
Salazar, Kayla Veronica	Northern New Mexico College	USG/Postbac	PADCAP/SSO	Whitaker, David Daleth, SSO
Sena, Joseph Paul	New Mexico State University	USG/Postbac	PADOPS/XIT-CSS	Lavy, April Lynn, XIT-CSS
Slone, Llewelyn Richard	University of California Los Angeles	USG/Postbac	PADOPS/SAE-3	Mconaha, Christopher Warren, SAE-3
Valdez, Julien Luis	University of New Mexico-Los Alamos	USG/Postbac	PADCAP/SSO	Rivera, Deb, SSO

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-26181

After The Click

We will be tracing the path of malware from the click on an email to its conclusion on a single host. We will be analyzing alerts, host logs, and network logs.

Engineering

Student(s): Brownfield, Ryan David; Fresquez, Brenden Joseph; Maldonado, Alexis; Trujillo, Ryan Isaac

Student Names	University/School	Program	PAD/Group	Mentor
Brownfield, Ryan David	Texas A&M University	GRA	PADOPS/NCS	Miko, David K, NCS
Fresquez, Brenden Joseph	Pojoaque Valley High School	High School	PADOPS/NCS	Montoya, Cindy N, NCS
Maldonado, Alexis	Texas A&M University	USG/Postbac	PADOPS/NCS	Trujillo, Julio B, NCS
Trujillo, Ryan Isaac	Espanola Valley High School	High School	PADOPS/NCS	Trujillo, Julio B, NCS

Category: Engineering

Type: Group Poster

LA-UR: LA-UR-18-26351

Teaching Simulator for Operators Based on Siberian Criticality Accident (1978)

The intent of the nuclear criticality simulators is to enhance the operators understanding of criticality safety concepts. This is done using a hands-on tool similar to that used in the operators work setting. A historical criticality accident is simulated using this tool in order to demonstrate criticality in a safe environment. The simulator will have black pucks to represent plutonium ingots and will have an ejection mechanism to simulate the thermal expansion that occurred during the criticality accident. The pucks will be in a can in a glovebox that is retrofitted with blue LEDs to simulate the blue flash.

Student(s): Brownfield, Ryan David; Fresquez, Brenden Joseph; Maldonado, Alexis; Trujillo, Ryan Isaac

Student Names	University/School	Program	PAD/Group	Mentor
Brownfield, Ryan David	Texas A&M University	GRA	PADOPS/NCS	Miko, David K, NCS
Fresquez, Brenden Joseph	Pojoaque Valley High School	High School	PADOPS/NCS	Montoya, Cindy N, NCS
Maldonado, Alexis	Texas A&M University	USG/Postbac	PADOPS/NCS	Trujillo, Julio B, NCS
Trujillo, Ryan Isaac	Espanola Valley High School	High School	PADOPS/NCS	Trujillo, Julio B, NCS

Category: Engineering

Type: Group Poster

LA-UR: LA-UR-18-26352

Nuclear Reactivity Simulator for Operator Criticality Safety Training

As Los Alamos National Laboratory continues to hire fissile material handlers (FMH) as pictured below, it is essential to train these workers and to show them how handling fissile material effects reactivity. The nuclear reactivity simulator provides an audio, visual, and tactile tool that familiarizes FMH workers with nuclear reactivity in a safe environment. Theremin technology simulates effect on reactivity from handling fissile material using the person's body as an electrical control. The 9.91 kg tungsten ball represents fissile material and clicking sounds increase as operator moves closer to tungsten ball. Cans with black pucks represent cans with plutonium-239 ingots.

Health & Safety

Student(s): Garcia, James Joseph; Lopez, Jeanette M; Lujan, Benjamin Patrick; Trujillo, Ariana Veronica; Valdez, Tamara Shayne

Student Names	University/School	Program	PAD/Group	Mentor
Garcia, James Joseph	UNM-LA	USG/Postbac	PADOPS/ASM-PM	Gonzales, Yvonne Christine, ASM-PM
Lopez, Jeanette M	Santa Fe Community College	USG/Postbac	PADOPS/SAE-4	Sanchez, Lea Danielle, SAE-4
Lujan, Benjamin Patrick	University of New Mexico	USG/Postbac	PADOPS/SAE-DO	Cisneros, Michael Paul, SAE-DO
Trujillo, Ariana Veronica	The University of New Mexico	USG/Postbac	PADOPS/ASM-PUR	Padilla, Mark Anthony, ASM-PUR
Valdez, Tamara Shayne	University of New Mexico	GRA	PADOPS/SI-ITPM	Gallegos, Linda A, SI-ITPM

Category: Health & Safety

Type: Group Poster

LA-UR: LA-UR-18-25231

Before the First Shot: Finding Technology for the Safety of the Public

Provide the ability to detect someone with the intent to become an active shooter prior to the first shot. At this point, technologies exist to detect aspects of this from a certain distance but none have been fully integrated. This project is to explore technologies available, research application at large facilities such LANL, and detail a plan to test candidate technologies.

Student(s): Logan, Amber Lee; Mang, Zachary Aaron

Student Names	University/School	Program	PAD/Group	Mentor
Logan, Amber Lee	University of New Mexico	USG/Postbac	PADOPS/OSH-OH	Sandin, Cynthia F, OSH-OH
Mang, Zachary Aaron	University of New Mexico	Post Masters	PADOPS/OSH-OH	Martinez, Adam, OSH-OH

Category: Health & Safety

Type: Group Poster

LA-UR: LA-UR-18-26091

Lift to Resist CVD: A Review of the Effects of Strength Training on Cardiovascular Disease Risk Factors

Cardiovascular disease (CVD) is the leading cause of death for both men and women, making its prevention and treatment a priority for doctors and researchers. While the risk of dying from a CVD-related event is partly genetic, there are several modifiable risk factors that can be influenced by lifestyle. These risk factors include hypertension, dyslipidemia, insulin resistance, smoking, and obesity. Traditionally, aerobic exercise (AE) has been prescribed to prevent CVD due to its ability to decrease inflammation while improving blood pressure, insulin sensitivity, and blood lipid profiles. More recently, however, the attention has shifted from aerobic to resistance training (RT), which not only has its own set of benefits, but is a more appealing mode of physical activity to novice exercisers. Therefore, the purpose of this study was to compile research that examines the effects of RT on the modifiable CVD risk factors (hypertension, dyslipidemia, insulin resistance, and obesity). Specifically, we found studies that focused on one of these risk factors at a time in order to fully understand the range of effects RT has across populations, frequency of training, and volume of training on each individual risk factor. Thirty studies were analyzed, after which we concluded that RT is a viable treatment and mode of exercise for the prevention of CVD. RT has been shown to decrease SBP, DBP, and MABP, effectively countering hypertension. It also increases skeletal mass, which increases RMR and leads to decreases in body weight, %BF, and WC. RT has many metabolic effects, too, such as improving HbA1c and blood glucose, along with LDL-C, TG, and TC. Its effects on insulin resistance, however, are still debatable. In the end, RT has a variety of benefits that counteract the risk factors for CVD, and the benefits are amplified when combined with classic AE.

Information Technology

Student(s): Anaya, Elizabeth Selena; Brown, Ashley Ann; Egan, Doug; Rodriguez-Acosta, Mireya; Zapata, Jannet

Student Names	University/School	Program	PAD/Group	Mentor
Anaya, Elizabeth Selena	Regis University	USG/Postbac	PADOPS/SI-ITS	Jaramillo, Jessica Marie, SI-ITS
Brown, Ashley Ann	Michigan Technological University	USG/Postbac	PADOPS/NIE-CS	Nolting, Walter William, NIE-CS
Egan, Doug	New Mexico Tech	USG/Postbac	PADOPS/NIE-IS	Merrigan, Dylan Russell, NIE-IS
Rodriguez-Acosta, Mireya	New Mexico Highlands University	GRA	PADOPS/SAE-3	Burkett, Travis, SAE-3
Zapata, Jannet	University of New Mexico	USG/Postbac	PADOPS/SI-ITPM	Gallegos, Linda A, SI-ITPM

Category: Information Technology

Type: Group Poster

LA-UR: LA-UR-18-25292

Green Network "Archeology" Project

The Green (unclassified open) network was created to house Laboratory computer systems that cannot reside on the Yellow (unclassified protected) network because they provide the following types of services: Servers that provide information or services to large external user bases that should not be granted access to the Yellow (including unauthenticated access to the general public); services that communicate with external systems using network protocols not supported by the Yellow firewall. The Green network has been in existence for approximately 20 years. Currently, the Green network does not have a management system that allows detecting outdated code or poor security practice. Because technology is constantly evolving, an outdated website or application could present vulnerabilities that enable Green network compromise. Since the Green network is Los Alamos National Laboratory's public facing network segment, it's highly important to keep all websites and repositories up-to-date, creating a well sustained public image for Los Alamos National Laboratory. Our goal is to create a comprehensive inventory of all websites, applications, and data repositories as well as analyze the data and make recommendations for possible remediation by identifying tools to survey and analyze the data.

Student(s): Jiron, Andres Isaiah; Rodriguez, Anthony Roy; Rodriguez, Sergio Robert; Tafoya-Montoya, Katelynn Marie Ice Blossom; Whitacre, Madeline Helene

Student Names	University/School	Program	PAD/Group	Mentor
Jiron, Andres Isaiah	University of New Mexico	GRA	PADOPS/XIT-TSS	Salas, Ben David, XIT-TSS
Rodriguez, Anthony Roy	Northern New Mexico College	USG/Postbac	PADOPS/XIT-ISS	Castaneda, Gerald Charles, XIT-ISS
Rodriguez, Sergio Robert	Utah Valley University	USG/Postbac	PADOPS/NIE-IS	Martinez, Mark L B, NIE-IS
Tafoya-Montoya, Katelynn Marie Ice Blossom	Arizona State University	USG/Postbac	PADOPS/XIT-CSS	Montoya, Jenelle Marie, XIT-CSS
Whitacre, Madeline Helene	University of New Mexico	USG/Postbac	PADOPS/SI-RMS	Carr, Alan Brady, SI-RMS

Category: Information Technology

Type: Group Poster

LA-UR: LA-UR-18-24891

Raspberry Pi Device Testing

The raspberry pi challenge is to research applications involving LANL main missions of weapons, global security, and science. The team will develop a plan to acquire, implement, and test a platform useful for future research applications within LANL mission space. The project team will have to develop an understanding of potential requirements, form a small team, develop roles, and ultimately evaluate the platform for a specific application to be determined by the team.

PADSTE

Individual Posters/Presentations

Biosciences

Student(s): Chau, Phuong Nguyen Uyen

Program: USG/Postbac

School: Smith College

PAD/Group: PADSTE/T-6

Mentor: Neale, Christopher Andrew, T-6

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26116

Drug Discovery by Chemical Similarity

Cancer is responsible for nearly 1 in every 6 deaths worldwide. Even though there are some available treatments for cancer such as surgery, chemotherapy, and radiotherapy, these treatments still have several limitations, such as their incomplete ability to distinguish between cancer cells and normal, healthy cells. As a result, these therapies can lower white blood cell levels, weaken the immune system, and damage the circulatory and digestive systems. As an alternative, we are developing drugs that will directly target the broken cellular machinery that is driving cancer without affecting healthy cells. These drugs will deactivate a mutant enzyme that causes relentless multiplication of cells (cancer cells). As part of a new anti-cancer drug discovery framework, I am developing computational tools to analyze the similarity between large sets of chemical compounds. We will use these tools to find classes of chemicals with structural similarities, which are expected to vary in their biological and chemical activities and their abilities to halt unregulated cell growth. By creating a fully connected chemical network that is informed by chemical similarity, this research will enable a simple, visible, and rapid search for groups of chemicals that are viable candidates for stopping cancer cell multiplication.

Student(s): Cirigliano, Elisa

Program: USG/Postbac

School: University of British Columbia

PAD/Group: PADSTE/B-11

Mentor:

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26410

Adaption of freshwater microalgae *Chlorella sorokiniana* to higher salinities for the production of biofuel

As petroleum and other fossil fuels are being depleted attention has focused on developing reliable renewable resources. Recently, there has been an increased interest in studying microalgae for biofuel production. Algae can be grown on a large scale on arid land with water that is not suitable for human or animal consumption, so it does not compete with freshwater resources or farmable land. An additional benefit of creating a commercial biofuel is that it would reduce the United States' dependence on foreign oil. Currently, some of the fastest growing, highest producing strains are freshwater microalgae, such as *Chlorella sorokiniana*. We have adapted several strains of *C. sorokiniana* to grow at a higher salinity at rates similar to, or better, than in fresh water. Culture growth was monitored by measuring optical densities and cell concentration. Additionally, cells grown in higher salinity media show an increased rate of lipid accumulation. This is measured by staining the neutral lipids of the cells and monitoring their fluorescence through flow cytometry. These lipids are the precursors for production of biofuel, hence a higher yield increases the efficiency and cost effectiveness of this technology. Fresh water production strains can be adapted to grow in higher salinity medium while increasing their growth and lipid production rates. This allows for the use of sea water, brackish water, or waste water for culture growth, reducing the dependence on fresh water needed for human consumption and agriculture.

Student(s): Finck, Anna Marie

Program: USG/Postbac

School: Concordia College

PAD/Group: PADSTE/B-11

Mentor: Barry, Amanda N, B-11

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-25454

Improving the Biomass Productivity of a Biofuel Production Strain, Nannochloropsis gaditana

Saltwater algae of the genus *Nannochloropsis* demonstrate potential as producers of biofuel precursors in part by high lipid content and the ability to withstand outdoor growing conditions. This project examines the growth of *Nannochloropsis gaditana*, a saltwater strain of brown algae, in the presence of three plant substrates (Corn Stover, Sugarcane Bagasse, and Switchgrass). We found that the growth of *Nannochloropsis gaditana* in the presence of plant substrates is faster, thus suggesting that *Nannochloropsis* has the ability to utilize lignocellulosic material as a carbon source. We investigated whether or not this improvement in growth was due solely to carbon utilization or to some other nutrient in the plant substrate. Furthermore, we examined the biochemistry of this activity, examining six native glycosyl hydrolase proteins.

Student(s): Hume-Dawson, Brittany Oremi

Program: USG/Postbac

School: Alabama State University

PAD/Group: PADSTE/B-10

Mentor: Ganguly, Kumkum, B-10

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26500

Emerging Issues in Treatment of Central Nervous System (CNS) Ischemic Disorders in Pediatric Population

Ischemic stroke is an important, yet understudied, contributor to morbidity and mortality in the pediatric population. The cost of pediatric stroke care is expensive given the lifetime expectancy need for clinical care in this patient population. Pediatric stroke may occur in as many as 1 in 4000 births and complications due to hypoxia/ischemia are common. Maternal and perinatal coagulopathy predispose to pediatric stroke with 30% of such events being due to thrombosis. The use of tissue type plasminogen activator (tPA) in children has been limited and its benefit remains unclear. The use of tPA in children is based on the assumption that studies in adults are generalizable, but the safety and efficacy of tPA in this setting have yet to be systematically investigated. A number of considerations should be contemplated when extrapolating the experience with tPA in adults to children, such as dosing, benefit/risk ratio, pharmacokinetics and therapeutic window.

Student(s): Jackson-Hundley, Val Zachary

Program: USG/Postbac

School: UC San Diego

PAD/Group: PADSTE/B-10

Mentor: Hovde, Blake, B-10

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26317

Identification of growth promoting bacteria for algae cultures

Algae biofuels are an ideal alternative to conventional fossil fuels as well as biofuel based crops like corn. This is because algae biofuel crops have a smaller environmental impact and significantly smaller land usage area while not requiring the use of current arable land. Despite these advantages, the algal biofuel production process is not yet efficient enough to make algal biofuels competitive with traditional fuels. Efficiency could be improved by identifying symbiotic algae-bacteria interactions and using these in biofuel cultures. Such interactions could allow for lowered nutrient input and faster biomass accumulation. By using microfluidics and flow cytometry to create controlled spaces for examining species reactions, several beneficial algal-bacterial interactions have been pinpointed. DNA sequencing has allowed the specific bacterial species involved in these interactions to be identified. Further testing is needed to describe the effect on growth that each bacterial species has individually on the algae.

Student(s): Jakhar, Shailja

Program: GRA

School: University of New Mexico

PAD/Group: PADSTE/C-PCS

Mentor: Mukundan, Harshini, C-PCS

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26393

Diagnosis of Tuberculosis by Direct Detection of Mycobacterial Lipoarabinomannan in Patient Serum

Almost one-third of the world's population is infected with tuberculosis (TB), the leading cause of death worldwide from single infectious agent ranking above HIV/AIDS. About 10% of those infected have a potential risk to develop active TB at some point in their life. Alarming, 40% of TB cases are either not diagnosed, or not notified to TB control programs, highlighting the limitations of current diagnostic platforms which are either inaccurate or inaccessible. A simple blood-based diagnostic would alleviate this problem which is the goal of our work. Lipoarabinomannan (LAM) is an amphiphilic tuberculosis biomarker carried by lipoprotein molecules such as HDL in blood. To detect presence of LAM in blood, we have developed a modified sandwich assay/lipoprotein capture assay (exploiting reliable antibodies supplied by FIND). We have evaluated sensitivity and specificity of the Lipoprotein capture assay in a blinded cohort of active TB patients along with other co-morbidities such as HIV from Uganda (n=48) and demonstrate performance in pulmonary and extra-pulmonary tuberculosis in this population, using an ultra-sensitive biosensor platform developed at the Los Alamos National Laboratory. We studied the corroboration of our measurement with sputum culture, blood culture and urinary LAM measurement as positive correlates, and identify serum lipoprotein concentrations as a key determinant in regulating concentrations of the biomarker in patient blood. Herein, our novel lipoprotein capture approach and the results of the validation study will be presented.

Student(s): Kelliher, Julia Mae

Program: USG/Postbac

School: Skidmore College

PAD/Group: PADSTE/B-10

Mentor: Dichosa, Armand Earl Ko, B-10

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-25665

Interrogating cell-cell interactions using gel microdroplet technology

Gel microdroplets (GMDs) are microsphere agarose beads intended to encapsulate viable cells for cultivation and downstream molecular assays. By addressing the fundamental principle observed in classical microbiology: that cells need other cells to thrive, LANL was the first to apply GMDs to advance the field of single cell genomics by recovering genomes of novel and ecologically relevant bacteria. Captured cells in GMDs can be monitored for growth via microscopy and tracked through flow cytometry, leading to the recognition of antagonistic and symbiotic relationships between the captured cells. To date, we have evolved the utility of GMDs to interrogate the complex cell-to-cell interactions occurring in diverse microbiomes – relevant to various sponsors including DoE, NIH, and NASA. Herein, I present several projects demonstrating GMDs' utility to elucidate the interactions between bacteria, fungi, algae, and their application to control diseases of the human gut microbiome in three LANL projects: 1. A study of the gut microbiome and how *Clostridioides difficile* infections can be treated with a therapeutic bacterial cocktail of gut microbes that naturally inhibit *C. diff* growth and replication (LDRD-ER) 2. Identifying the bacterial-fungal interactions in the rhizosphere and their impact to soil ecosystems and nutrient cycling (DoE-SFA) 3. Recovering symbiotic bacteria of Antarctic tunicate organisms that may have anti-cancer properties (NIH-R21) GMDs are an extremely versatile tool in a biological laboratory, and their capabilities and applications are still being uncovered.

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PAD/Group: PADSTE/B-11

Mentor: Dale, Taraka, B-11

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-25937

Enhancing monooxygenase efficiency for the production of polymer precursors using 'smart' microbial cell technology

Monooxygenases are enzymes that catalyze oxygenation reactions, or reactions where an oxygen atom is inserted into organic substrate through electrophilic and nucleophilic interactions. These are capable of catalyzing diverse reactions, from hydroxylations to halogenations. In our project, p-hydroxybenzoate hydroxylase (PobA) is our monooxygenase of interest from *Pseudomonas putida*. The substrate required by PobA is found in lignin, an organic polymer and constituent of plant cell walls. Although lignin is considered an industrial waste, lignin as a substrate source plays a substantial role in the production of muconate, a precursor for nylon and plastics with a market value of 40 billion dollars. This conversion step is crucial for lignin valorization. PobA utilizes flavin adenine dinucleotide (FAD) as a coenzyme and nicotinamide adenine dinucleotide phosphate (NADPH) as an electron donor in the hydroxylation of 4-hydroxybenzoate (4HB) to produce protocatechuate (PCA or 3,4-dihydroxybenzoate). PCA is a key intermediate in the production of muconate or beta-ketoadipate, precursors for polymers and plastics. Research from groups shows accumulation of 4HB in the bioconversion, indicating PobA as a bottleneck enzyme in the synthetic metabolic pathway. Thus, the focus of my work is to improve the enzymatic activity of PobA, thereby, improving the conversion of 4HB to PCA. In order to accomplish this, I will apply molecular biology techniques and knowledge of enzyme structures gained throughout my internship. I will carry out select mutations derived from homologous sequences in the substrate binding pocket of PobA. A mutagenic library of pobA gene is created and transformed in *P. putida* strain. The PobA variant is evaluated using 'smart' microbial cell technology, where enzymatic activity correlates with fluorescence response, allowing for the selection of a good performer by visualization on agar plates or sorting using flow cytometry. The work is part of a multi-national laboratory effort (Agile Biofoundry) for advanced biomanufacturing.

Student(s): Lakis, Isabelle Marie

Program: USG/Postbac

School: New Mexico Institute of Mining and Technology

PAD/Group: PADSTE/B-10

Mentor: Cui, Helen Hong, B-10

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26107

Comparing DNA Recovery from Cotton, Nylon, and Rayon Swabs Used for Environmental Metagenomic Analysis

Metagenomics is the study of all genetic material within a microbial community. In practice, metagenomics involves the categorization of microorganisms, a determination of relative abundance, and an evaluation of total genetic content within a community structure. These microbial communities evolve and adapt to their surroundings, reacting to changes in their environment. It is widely acknowledged that many bacteria cannot be cultured in a laboratory setting, but metagenomics allows us to observe communities by extracting DNA directly from samples eliminating culturability concerns. The bacteria within a community are extremely diverse, and it is difficult to determine a general technique for sampling from different environments. One of the common methods used is swabbing a target area with a dampened fiber tip. Swabs come in many sizes and are made of materials both natural and synthetic. Some swabs have tips wrapped in fibrous materials; others are flocked to provide more uniform texture. Both the texture and material of swabs used can have a significant impact on the results of bacteria or spore collection and culturing. However, in the context of DNA recovery, these properties have only been studied in a limited capacity. In order to address this gap in knowledge and maximize the DNA recovered from samples, performed an experiment exploring the DNA recovery from various swab types – wrapped cotton, wrapped rayon, and flocked nylon – on different environmental surfaces. Swab samples were collected from surfaces including trees, rocks and buildings. The DNA was then extracted from the sample using a nucleic acid extraction kit and analyzed. To assess our results, we will use a fluorometer to quantify concentrations of extracted DNA, perform quantitative polymerase chain reactions to ascertain the quality of DNA, and will use statistical analysis to compare the DNA recovery of each swab type on various surfaces.

Student(s): Lenz, Kiersten Danielle

Program: GRA

School: University of New Mexico

PAD/Group: PADSTE/C-PCS

Mentor: Mukundan, Harshini, C-PCS

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26367

Adaptation of centrifugal microfluidic techniques for blood sample processing to detect *Francisella tularensis*

Early and accurate detection of bacterial infections is necessary to guide treatment decisions and prevent the evolution of antibiotic resistance.¹ Our team at LANL has developed a waveguide-based optical biosensor to quickly detect biomarkers indicative of infection from patient samples at the point-of-care.² However, the bacterial biomarkers targeted by these assays are lipids, and their amphiphilic biochemistry causes them to be sequestered by host lipoprotein carriers.³ We have developed a novel and sensitive detection method—membrane insertion—for the direct measurement of amphiphilic biomarkers. For this, however, the patient sample must first be processed to separate serum from blood, and then the lipids must be extracted from their lipoprotein carrier complexes in serum.³ Current sample processing methods require highly trained personnel and extensive laboratory procedures. We have adapted previously-developed centrifugal microfluidic techniques to automate serum separation from blood.⁴ The automation of sample preparation saves time and ensures user safety, an important consideration when handling potentially infectious human blood.⁵ We fabricated a centrifugal microfluidic device from plasma-treated acrylic and polycarbonate that is effective at separating serum from blood. The device is also able to move serum into its own reservoir via a siphon for further processing. We are working on validating our serum separation device using enzyme-linked immunosorbent assays to confirm that the biomarker of interest is retained in the sample and is not adsorbed to the surface of the device. Initially, we are working with a vaccine strain surrogate of *Francisella tularensis*, a Tier 1 Select Agent with biological warfare potential. This step evaluates the suitability of the device engineering and surface chemistry for separation of amphiphilic targets, as has never been shown before. Moving forward, we plan to fully automate the entire lipid isolation process on a centrifugal microfluidic device, which will be integrated with our Universal Bacterial Sensor.

Student(s): Mahesh, Riya

Program: USG/Postbac

School: University of Texas at Austin

PAD/Group: PADSTE/T-6

Mentor: Hengartner, Nick, T-6

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26416

Identifying Gene Expression Signatures of Cancer Driver Mutations in R

Cancer is the second leading cause of death in the US. Since both the incidence and cure of cancer have a genomic component, there is an opportunity to individualize treatment. To learn how treatment and genomics are linked, the National Cancer Institute (NCI) and other organizations have developed immortal cancer cell lines to systematically test drug response, and related the assays to gene expression data. However, this drug response data is not available for patient tumor data from The Cancer Genome Atlas. We seek to discover the gene expression signatures of known driver mutations in order to predict drug response on the patient tumor data. We calculate the posterior probability that each gene is affected by the driver mutation and multiply the probability by the sign (+/-) of the gene expression data in order to determine whether the gene is upregulated or downregulated. These probabilities and their respective genes can then be plotted on a KEGG pathway using the pathview package in R.

Student(s): Martinez, Savannah Abelina

Program: USG/Postbac

School: New Mexico State University

PAD/Group: PADSTE/B-10

Mentor: Dichosa, Armand Earl Ko, B-10

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26218

A Novel Method for Monitoring Cell-to-Cell Interactions

Considerable evidence suggests that interactions between the bacterial and fungal constituents of the soil microbiome surrounding plant roots (the rhizosphere) are vital to carbon fluxes, nutrient cycling, and plant productivity. Monitoring and imaging the growth of fungi in proximity with key bacteria is important to understand these bacterial/fungal interactions. However, the availability of non-invasive tools to directly observe these fundamental interactions are limited. To address this limitation, we are developing a novel method to observe these interactions by using gel microdroplets (GMDs). The GMDs were employed to co-capture a single fungal spore with a bacterial cell. We hypothesize that the presence of a rhizosphere bacterium will have an observable effect on fungal spore germination; we are testing this using our method to create a microscope slide with agar pads that enable the cultivation and monitoring of a single GMD through time. Single GMDs containing the fungal and bacterial cells were sorted onto an agar pad using a flow cytometer. We are optimizing methods to create these agar pads to improve the visualization of the GMDs and to preserve them for repeated microscopic observations of fungal growth. This new method for real-time observations of co-captured fungal spores and bacteria can also be applied to cell-to-cell interactions between other types of organisms.

Student(s): Mensah, Caroline

Program: USG/Postbac

School: Alcorn State University

PAD/Group: PADSTE/B-10

Mentor: Ganguly, Kumkum, B-10

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26503

Understanding the Radiation Induced Bystander Effect (RIBE)

Ionizing radiation is energy transmitted via X rays, gamma rays, beta particles, alpha particles, neutrons, protons, and other heavy ions. When exposed to ionizing radiation, large molecules such as nucleic acid and proteins in the organisms will be ionized or excited. This may cause changes in the molecular structures which then affect the function and metabolism of the cells. Laboratory experiments have demonstrated that ionizing radiation can cause breakage of the DNA chain (double strand break, DSB) or can deter cell replications. Radiation induced bystander effect (RIBE) was found in 1990 and challenged the conventional dogma that no effects were expected in cells that had not been exposed to radiation. We studied the mechanisms underlying RIBE, which enlightened us on directions to radiation protection against low-dose environment radiation as well as during radiotherapy. RIBE brings potential hazards to normal tissues in radiotherapy, and imparts a higher risk from low-dose radiation. Detection with proteins related to DNA damage and repair, cell cycle control, proliferation, etc. have enabled rapid assessment of RIBE in a number of research system.

Student(s): Mettler, Jacquelyn Gloria

Program: USG/Postbac

School: Northern Arizona University

PAD/Group: PADSTE/B-10

Mentor: Starkenburg, Shawn Robert, B-10

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26106

CRISPR-Directed Editing of Photoreceptor Genes to Improve Biomass Accumulation in Microalgae

The current estimate of algal biofuel production costs, utilizing all current best practices and scaled to industrial levels, are \$8.50 per Gallon of Gasoline Equivalent (GGE). However, greater than 75% of that cost comes from the algal feedstock production and harvest, whereas only a minimal portion of the cost comes from processing and refinement of the biocrude. By increasing algal yields and rates of harvest for algal biofuel feedstocks, the production costs can be significantly reduced. To achieve a significant yield increase in algal biomass, we propose carrying out both a targeted gene knockout of an algal photoreceptor (phototropin) and targeted gene replacement with a chimeric plant photoreceptor (neochrome). Phototropins are a class of highly conserved photoreceptors used by photosynthetic organisms to sense blue light and, when activated by light, enable plants to maximize the capture of photosynthetically active radiation. Preliminary data shows that knocking out phototropin alone can increase biomass production in the model green alga *Chlamydomonas reinhardtii* two-fold. Therefore, knockout of phototropin in a commercial production level algal species may greatly improve yields. The gene proposed for targeted insertion, neochrome, is a chimeric photoreceptor that contains both phototropin and phytochrome photoreceptor domains and is able to perceive blue/red/far red light exhibited in shaded conditions. We anticipate that photosynthetic efficiency will be improved and result in an additive increase in the biomass accumulation rate in rapidly changing light environments. Both of the methods described have the potential to greatly improve the biomass production or photosynthetic efficiency of production level strains.

Student(s): Pane, Anthony Joel

Program: USG/Postbac

School: University of Rochester

PAD/Group: PADSTE/T-CNLS

Mentor: Neale, Christopher Andrew, T-6

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26168

A Biological Master Key: How an Unstructured Protein Takes Shape

Our bodies have natural defenses against cancer. The p53 tumor suppressor protein is one such defense which prevents the growth of cancerous cells. Mutations to the p53 protein account for more than 50% of human cancers, making this a widely studied protein. Like all proteins, p53 is a biomolecule that performs its function due to its shape and chemical properties. However, unlike many other proteins, an active region of p53 does not have one single defined shape. This region, called the C-terminal domain (CTD), interacts with a number of biomolecules to perform its tumor suppressing function. Experiments show that the p53-CTD takes on different shapes depending on which of these biomolecules it binds to. Interestingly, the region is unstructured while not interacting with another molecule. This is roughly analogous to an amorphous key that fits into different locks by taking on different shapes. Experiments show that the p53-CTD does form to different shapes, yet there is much debate as to the mechanism of these changes. While the p53-CTD could randomly take a shape that will fit to the biomolecule, the biomolecule could also be changing the shape of the p53-CTD. In other words, does the key randomly take the shape of the lock or does the lock act like a mold to change the shape of the key. In this work we attempt to answer this question using computer simulations of the p53-CTD. We use temperature replica exchange to allow the protein to quickly transition between structures. Using this method of simulation on both the protein by itself and biomolecules will help us better understand how the C-terminal domain of p53 tumor suppressor protein is able to interact with multiple different binding partners to prevent the growth of cancer cells.

Student(s): Pedersen, Christine Ashley

Program: USG/Postbac

School: University of California, Merced

PAD/Group: PADSTE/C-PCS

Mentor: Mukundan, Harshini, C-PCS

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-25980

Application of Long-Term Air-Stable Lipid Bilayers for Waveguide-Based Biosensors

The Biosensor team at Los Alamos National Laboratory strives to detect pathogens using a biosensor system for rapid diagnosis. Biosensor systems utilize molecules to detect the presence of pathogens using physiochemical optical transducers. Transducers surfaces are functionalized using lipid bilayers, allowing for attachment of recognition elements for specific attachment of recognition elements, which include antibodies to identify targets of interest, such as pathogenic organisms. Supported lipid bilayers (SLBs) can only tolerate a narrow range of handling and environmental conditions, thus introducing constraints of structural instability and making long-term storage difficult to achieve. In order to overcome these limitations, our team is working to create stable surfaces by utilizing suitable bilayer precursors. PSLB are produced by rupturing self-assembled lipid vesicles to a surface, followed by UV-initiated polymerization forming covalent networks that cross-link within the bilayer, enabling long-term storage. We will compare the performance of these PSLBs to our standard DOPC-based systems using the waveguide-based optical biosensor. This work will pave a way for an affordable and deployable sensor element, and a broadly applicable strategy for biodetection.

Student(s): Silver-Isenstadt, Maya Sage

Program: USG/Postbac

School: University of Maryland College Park

PAD/Group: PADSTE/B-11

Mentor: Dale, Taraka, B-11

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-25958

Altering Substrate Specificity of Glucose Dehydrogenase for Increased Xylose Utilization in *Pseudomonas putida*

The United States annually produces over 120 million tons of corn stover from agricultural plant waste. Corn stover is composed of cellulose, hemicellulose, and lignin: all of which can be converted into viable and renewable feedstocks for microbial production of commodity chemicals, currently sourced from petroleum. We are working with *Pseudomonas putida* which has been engineered to produce cis-cis muconate (CCM). This molecule is an immensely valuable industrial precursor to many plastics. However, these industrially relevant strains have trouble taking in and metabolizing xylose which is the second most abundant sugar in biomass. The goal of this project is to engineer *P. putida* to effectively utilize xylose for the production of CCM. The conversion of glucose to gluconate that diverts the carbon away from CCM production pathway is catalyzed by the enzyme glucose dehydrogenase (*gcd*). A *gcd* knockout strain resulted in high muconate yield yet it had the overall side-effect of lowering cell performance due to slow growth. However, *gcd* is promiscuous and has the potential to utilize xylose as a substrate along with glucose. Altering *gcd* expression levels and/or creating a substrate-specificity switch will hopefully maintain the muconate yield while improving cell growth rate. The activity of the pathway can be linked with a biosensor which binds with the product of the *gcd* pathway and activates a green fluorescent protein (GFP) gene. Individual cells can be screened and sorted based on fluorescence levels. This technology will be utilized for high-throughput screening for best performing strains with high CCM production and robust growth. Creating plastics in a carbon-neutral cycle will not only be environmentally beneficial but will allow the United States to become less dependent on foreign countries for petroleum imports.

Student(s): Small, Jacori Alleace

Program: USG/Postbac

School: Delaware State University

PAD/Group: PADSTE/B-10

Mentor: Ganguly, Kumkum, B-10

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26501

Multi-Drug Efflux Pumps and Quorum Sensing Systems in *Pseudomonas aeruginosa*

Multi-drug resistance (MDR) efflux pumps belonging to the nodulation cell division (RND) family are important in conferring resistance to many drugs and antibiotics. However, these pumps are not there just for efflux of drugs. The very drugs that are pumped out by these efflux pumps can also induce expression of the efflux genes/proteins. In addition, the MDR efflux pumps transport out quorum-sensing (QS) molecules, which are known to induce expression of several genes including those related to biofilm formation, virulence, and efflux. Efflux pumps in *Pseudomonas aeruginosa* control biofilm formation and virulence thereby conferring additional resistance to drugs and also resistance against host innate immune defense. We performed several measurements on nascent and mature stages of biofilm both with ciprofloxacin (1mg/ml) and without it. These measurements included: (i) size and (ii) biofilm survival and drug efflux; (iii) expression of genes related to biofilm formation, virulence, and efflux by real-time qPCR, (iii) synthesis of pyocyanine and rhamnolipid, which are markers for biofilm and virulence; (iv) activity of the virulent enzymes, elastase and chitinase; and (v) neutrophil killing to monitor abrogation of innate immune defense.

Student(s): Van Tassel, Brett Thomas

Program: UGS/Postbac

School: Ramapo College of New Jersey

PAD/Group: PADSTE/B-10

Mentor: Shakya, Migun, B-10

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-26483

Understanding the evolution of Burkholderia genera through signature sequences

Genomic Origin Through Taxonomic CHAIenge (GOTTCHA) is a read based taxonomic profiler for metagenomic analysis. It maps reads to a unique database of signature sequences representing a taxonomic level. Signature sequences are extracted from corresponding genomes through iterative comparison and removal of similar regions from genomes. This process is repeated until all unique pairs are compared. Here, we focused specifically on Burkholderia genus and characterized their signature sequences to understand their evolution. First, we gathered metadata of signature sequences like what gene they code for and what are their specific functions. Second, we compared signature sequences among different species of Burkholderia to find the similarities and differences in potential phenotypes based off corresponding signature sequences. Lastly, we collated these different pieces of information and listed potential genes or phenotypes that explain the evolution of Burkholderia.

Student(s): Wright, Kimberly Theresa

Program: GRA

School: University of New Mexico

PAD/Group: PADSTE/B-11

Mentor: Dale, Taraka, B-11

Category: Biosciences

Type: Individual Poster

LA-UR: LA-UR-18-22167

Overexpression of the vacuolar proton-pumping pyrophosphatase, AVP1, increases starch accumulation in *Picochlorum soloecismus*

Picochlorum soloecismus (hereafter *Picochlorum*) is a green halotolerant microalga with fast growth rates, moderate starch/lipid accumulation, and is amenable to genetic engineering. We set out to increase carbon storage in *Picochlorum* by overexpressing its native vacuolar proton-pumping pyrophosphatase, AVP1, which has been shown to increase biomass in plants. We hypothesized that by overproducing AVP1 in microalgae, the consequent increase in the vacuolar proton gradient, and the decrease in inhibitory pyrophosphate, would increase ATP levels and photosynthetic efficiency. Ultimately, this results in an increase in carbon storage molecules. The expression of AVP1 and Sh-ble was driven by native RbcS and TELF promoters/terminators, respectively, and were inserted into the genome via electroporation. Gene integration and expression were confirmed by PCR, sequencing, and RT-PCR. AVP1 overexpression lines were compared to wildtype by growth, light and electron microscopy, biochemical composition, and oxygen evolution. Although we continue to characterize these strains, our preliminary data shows that AVP1 mutants accumulate more starch than the wild type, without significantly affecting growth. These results suggest that AVP1 overexpression can benefit algal biofuel production strains by increasing the overall carbon storage of *P. soloecismus*.

Chemistry

Student(s): Arafat, Omar I

Program: USG/Postbac

School: UCLA

PAD/Group: PADSTE/C-IIAC

Mentor: Sutton, Andrew, C-IIAC

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-26427

A Furfural Free For All

A Furfural Free For All Arafat, Omar Fawaz I; Sutton, Andrew; Kubic, William Louis; Yang, Xiaokun Affiliations: MPA11 CIIAC AET-2 By converting biomass into fuels and higher-value chemicals, the world can reduce its dependence on oil and other vanishing natural resources. Here, we design and prove a high-yielding two-step procedure to convert a side product of corn ethanol production, corn bran, to furfural, generating a high-value chemical at a third of the current cost. The DOE identified Furfural is one of the top bio-derived platform chemicals. The suggested process can either be retro-fitted into current corn Ethanol plants or built into new ones..

Student(s): Eiroa Lledo, Cecilia

Program: GRA

School: Washington State University

PAD/Group: PADSTE/C-AAC

Mentor: Olson, Angela Christine, C-AAC

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-25788

Ni-57 isolation and characterization from neutron activation products, fission products and soil

The quantitative separation of metals from different matrices is essential for an accurate determination of metal concentrations present in the environment. Heavy metals are found in natural and contaminated soils and pose a health hazard if they enter the food chain by the uptake of contaminated plant matter or water. Obtaining precise metal concentrations from soil samples is essential for environmental tracking and remediation. The quantification of nickel (Ni) in complex environmental samples poses a challenge due to its chemical behavior. Ni behaves similarly to other metal ions, making it difficult to achieve complete separation from metals like Co, Cu or Fe. Previous Ni separation methods consist of extensive steps, with the need for high temperatures and the combined use of several hazardous chemicals. The separation method proposed in this work allows for the accurate isolation of Ni from a soil matrix containing other heavy metal contaminants. The rapid separation, isolation and characterization of Ni-57 from a complex matrix was achieved in 3 hours with an 80% chemical yield, without heating the samples. Gamma spectroscopy data from several separation experiments were evaluated to determine a detailed separation scheme, with information on each step of the separation process. Based on the results of the separation profile, optimization of individual steps was conducted using stable carriers and ICP-OES analysis.

Student(s): Frankle, Rachel Katherine

Program: USG/Postbac

School: Royal College of Surgeons in Ireland

PAD/Group: PADSTE/B-11

Mentor: Yoder, Jacob Luther, B-11

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-26057

Fieldable chemical analysis using J-coupled spectroscopy at earth's magnetic field

With the growing threat of hazardous chemical agents, there exists an ever increasing risk to national and global security. Thus, the need for rapid identification of such agents becomes necessary to respond to incidents where such chemical agents are deployed. At present, systems used for the immediate identification of chemical agents in the field are limited; current analysis methods require for the chemical agents to be transported to a lab located far from the incident site. This project aims to develop a portable device used to identify the J-couple spectra of such chemical agents. Molecules exhibit unique homo- and heteronuclear J-couplings between nuclei which are used to identify their structures, and these J-couplings can be measured using NMR spectroscopy at earth's magnetic field. At such low magnetic fields, the J-couplings are subject to additional splitting from neighboring nuclei, leading to more detailed information lost at high fields. Hence, this project utilizes earth field NMR to detect these J-couplings and eliminates the need for larger superconducting magnets that operate at high fields, enabling the development of a portable device that can be taken into the field. We collect J-couplings at earth's magnetic field as a proof of concept of such a fieldable system to be scaled down into a microfluidics system. However, NMR spectra collected at this low magnetic field suffers from diminished resolution and signal intensity, making data acquisition and analysis challenging; this problems is also compounded by the sample size in a microfluidics system. To overcome these challenges, we are exploring methods of pre-polarization using 1T Halbach magnet and dynamic nuclear polarization. By employing pre-polarization with earth's field NMR measurements, this system has the potential to solve the critical problem of quickly identify chemical agents in the field, thus enabling the proper response to any chemical threat.

Student(s): Hjelvik, Elizabeth Anne

Program: USG/Postbac

School: University of New Mexico

PAD/Group: PADSTE/C-PCS

Mentor: Anderson, Aaron S, C-PCS

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-25436

Optimization of plastic functionalization for applications in biosensors

Student(s): Koppi, Mackenzie Lynn

Program: USG/Postbac

School: UNM-LA

PAD/Group: PADSTE/C-NR

Mentor: Margiotta, Cheriece, C-NR

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-26446

Analysis of Four Decades of Background Spectra from a Lithium-Drifted Germanium Detector

Using the program PeakEasy, specific data from over one thousand archived background counts on C76 spanning from 1975 to 2018 were analyzed. Each spectrum was calibrated to 1 keV/channel at 2048 channels. Peak energy, total number of counts, net peak area, full width at half maximum, and error margin data was taken from three regions of interest (ROIs) including the annihilation peak at 511 keV, the ^{56}Fe (n,n') peak at 846.7 keV and the 40K peak at 1460 keV. This information was used to compare and analyze the historical background data to current backgrounds from C76.

Student(s): Mercer, Emily Rachel

Program: USG/Postbac

School: Whitman College

PAD/Group: PADSTE/C-IIAC

Mentor: Sutton, Andrew, C-IIAC

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-25814

Performance Advantaged Renewable Fuels by Design

The United States' dependency on foreign petroleum-derived fuels is not only an issue of national energy security, but also one concerning the future of our environment. There have been substantial developments in synthesizing fuels from domestic biological feedstocks, such as ethanol; however, the use of terpenes (components of essential oils coming from a wide range of plants) and their derivatives as biologically derived fuels has yet to be widely explored. Specifically, myrcene (C₁₀) is an industrially available monoterpene that has similar reactivity to the unsaturated hydrocarbons of oil and gas. Working with myrcene as a building block for high performance fuels, we will use heterocoupling processes to generate hydrogenated myrcene dimers for fuel property testing. To produce high performance fuels we aim to increase the combustion efficiency as well as the energy density. Thus, we have a goal of increasing both the cetane number (CN), which is an indicator of combustion speed of diesel fuel and an important factor in determining fuel quality, and the lower heating value (LHV), which typically decreases with increasing CN. Furthermore, this heterocoupling approach will enable fuel property improvements and further understanding of the effects of structural changes on improving yield sooting index (YSI),

Student(s): Nisbet, Haylea Dawn

Program: GRA

School: McGill University

PAD/Group: PADSTE/EES-14

Mentor: Migdisov, Artaches, EES-14

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-25964

An experimental investigation into the behavior of thorium in aqueous solution at elevated temperature

Thorium, the most abundant actinide in the earth's crust, has long been considered a potential energy-producing component to the nuclear fuel cycle. Although under-appreciated in the past, there has been growing interest in the development of thorium-based nuclear power due to its many advantages over uranium: 1) thorium is highly resistant to nuclear proliferation; 2) its ability to compliment the uranium/plutonium cycle and 3) its lower level of waste production. On another hand, thorium is considered a radioactive contaminant in mining practices, in particular with mining of the rare earth elements (REE). Whether it be interest in nuclear energy or exploration for Th-depleted ore deposits, it is crucial to understand the behavior of thorium in hot aqueous systems. The major limitation in modeling thorium is a lack of thermodynamic data for thorium species in aqueous solution at elevated temperatures, as the current database is largely restricted to ambient temperature. Presented are crucial high-temperature thermodynamic data for thorium species in chloride and sulfate-bearing aqueous solutions derived from solubility experiments performed at temperatures up to 250°C and saturated water pressure. Further, preliminary models describing the mobility of thorium in REE-hydrothermal systems will be presented.

Student(s): Rijal, Biswas

Program: GRA

School: University of Florida

PAD/Group: PADSTE/T-CNLS

Mentor:

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-26394

Theoretical studies on surface chemistry of actinide dioxide (AnO₂)

The fluorite structured actinide dioxides (AnO₂) are the most common nuclear fuels that are widely used in nuclear reactors for generation of electricity. Understanding surface chemistry of AnO₂ is crucial for the safe storage of spent nuclear fuels as well as the treatment of nuclear wastes. Our knowledge of AnO₂ surfaces is extremely limited due to the challenges in handling radioactive and toxic actinides in experiments, and the complexity in treating strongly-correlated 5f electrons in theory. A handful studies have been undertaken on UO₂ and PuO₂ surfaces, while the rest of the AnO₂ series have not been explored. Therefore, in this study, we present the first systematic study on surfaces of the AnO₂ across the series (Thorium to Californium). We focus on surface energies as a function of surface structures that will lead to better understandings of surface chemistry.

Student(s): Russell, Christopher Stephen

Program: GRA

School: Brigham Young University

PAD/Group: PADSTE/T-1

Mentor: Kress, Joel David, T-DO

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-25107

Improving Full-Scale Models of New Carbon Capture Technologies with Uncertainty Quantification

Carbon Capture technologies for combustion power plants aim to remove CO₂ from flue gas. One such technology is the novel CO₂-Binding Organic Liquid (CO₂BOL) process developed at the Pacific Northwest National Laboratory. The process utilizes their anhydrous CO₂BOL solvent in place of amine mixtures to reduce the energy penalty. A full-scale model based on NETL's Case 10 power plant is projected to produce 7-16% more net electric power over a traditional MEA system for the same plant. These full-scale model predictions are promising, however they are difficult to validate using only bench-scale data. Errors in both the measurements and models need to be considered in addition to uncertainties from up-scaling. Uncertainty quantification (UQ) is a statistical framework used to better understand these uncertainties as well as data gaps in models. By constraining models to data, distributions of model parameters are estimated and then propagated through the model to obtain distributions of key outputs such as carbon capture percent, energy penalty, etc. The UQ results aid the design of experiments (DoE) which identifies data gaps. Using UQ and DoE effectively can reduce the development time of new carbon capture by years and save money on the path to a pilot, and ultimately full-scale, plant.

Student(s): Staun, Selena Lee

Program: GRA

School: University of California Santa Barbara

PAD/Group: PADSTE/C-IIAC

Mentor: Gaunt, Andrew James, C-IIAC

Category: Chemistry

Type: Individual Poster

LA-UR: LA-UR-18-25997

Assessing Covalency in Transuranic Molecules

Nuclear energy is a significant component of electricity production in the United States. Used nuclear fuel, waste from the nuclear reactors, is comprised of uranium, fission products (both stable and highly radioactive), and other actinides (Pu, Np, Am, Cm). Various separation schemes for these different components are being considered as part of possible strategies to process and dispose of this highly radioactive waste. One way to separate lanthanides from actinides (and actinides from each other) is through differences in covalency in the metal-ligand bonding. Experimentally, covalency can be probed by NMR spectroscopy coupled with syntheses and structural characterization of target molecules containing multiple bonds with an inherent degree of covalent character. Synthetic protocols developed for uranium and thorium are being extended to neptunium and plutonium taking advantage of unique radiological facilities at Los Alamos to generate novel examples of rare transuranic molecules containing multiply bonded functionalities.

Computing

Student(s): Butts, David Joshua

Program: GRA

School: Michigan State University

PAD/Group: PADSTE/CCS-2

Mentor: Cooley, James Hamilton, CCS-2

Category: Computing

Type: Individual Poster

LA-UR: LA-UR-18-25375

Agent Based Techniques for Multi-Threat Environment Managment

After extreme events, cities often are left in a multiple threat environment. The effects of such extreme events and their interactions with each other and the environment can be difficult to represent mathematically. More so human's reactions to multiple threats can be difficult to mathematically model, with some of the most insightful behavior being missed by not using agent-based techniques. This project, using agent based modeling, simulates the aftermath of an extreme event in a city, and aims to optimize evacuation, rescue, and clean up protocols for civilians and emergency workers.

Student(s): Hirschhorn, Jacob Aaron

Program: USG/Postbac

School: University of Florida

PAD/Group: PADSTE/MST-8

Mentor: Matthews, Topher, MST-8

Category: Computing

Type: Individual Poster

LA-UR: LA-UR-18-26398

Implementation of CALPHAD-Based Phase Prediction for BISON's Metallic Fuel Model

The constituents of uranium-plutonium-zirconium (U-Pu-Zr) metallic nuclear fuels diffuse in response to concentration and temperature gradients in a process known as constituent redistribution. Macroscopic heterogeneities develop in the fuel during operation as the constituents diffuse. These heterogeneities correspond to phases with different crystal structures, compositions, and thermo-mechanical properties. Constituent redistribution affects reactor safety and fuel performance and must be accounted for to facilitate safe and efficient development of U-Pu-Zr fuels. The BISON Metallic Fuel Redistribution Model is currently being used to study and predict this behavior. Los Alamos National Laboratory contributes to development of the model as part of the Department of Energy's Advanced Fuels Campaign. BISON uses a simplified four-phase model based on a single (U-Pu)-Zr pseudo-binary phase diagram to predict the stable phase(s) throughout the fuel. Binary interdiffusion of U and Zr is then modeled using phase-specific diffusion parameters, which are calibrated and validated using post-irradiation examinations of U-Pu-Zr fuels. Current BISON predictions agree with experimental observations qualitatively, but refinements are necessary to increase model accuracy and certainty. The current work involves refinement of the model's thermodynamic description of the system and identification of constraints for recalibration of its diffusion parameters. Thermodynamic assessments of the system are used in conjunction with pycalphad libraries to add a fifth phase to the model and describe phase equilibria over wider ranges of compositions and temperatures. Published phase diagrams and diffusion data are reviewed to identify appropriate levels of composition dependence for each diffusion parameter, helping to maximize calibration accuracy and efficiency. Finally, predictions made using the refined model are compared to previous results to study the effects of phase diagram simplification on model calibration. These studies will enhance our understanding of the mechanisms underpinning constituent redistribution in U-Pu-Zr fuels and our ability to model the phenomenon using BISON.

Student(s): Jaganathan, Divya

Program: Post Masters

School: Brown University

PAD/Group: PADSTE/NSEC

Mentor: Petersen, Mark Roger, CCS-2

Category: Computing

Type: Individual Poster

LA-UR: LA-UR-18-26018

Optimizing Computational Performance of Variable Resolution Meshes through a Weighted Domain Decomposition

The Model for Prediction Across Scales (MPAS) – Ocean is an unstructured model with variable resolution capability that addresses the computational demand of high-resolution modeling of ocean in regional domains of interest. MPAS-Ocean is able to simulate fine scale features regionally at a fraction of the computational cost of a corresponding global high resolution simulation. To implement distributed-memory parallelism in MPAS-Ocean, the initial grid is partitioned into sub-domains using the graph-partitioning tool-METIS. The sub-domains are then assigned to individual processors. We assess the parallel performance by measuring the computational throughput defined by the Simulated Years Per Day (SYPD) metric across different processor counts. We observe deviation in performance scaling from theory at large processor count owing to increased communication overhead relative to computations between processors. We propose to address this deviation by re-assessing load distribution across processors. In the present model, the partitioning follows uniform decomposition of grid across processors assuming uniform work load in all sub-domains. However, we recognize some tasks in the model that scale differently with the depth. We thus present a weighted mesh partitioning method based on the variable domain depth in order to ensure load balancing on every processor and thereby potentially improving parallel efficiency at large processor count (~ 10k).

Student(s): Li, Bowen

Program: GRA

School: University of Michigan

PAD/Group: PADSTE/T-CNLS

Mentor: Bent, Russell, T-5

Category: Computing

Type: Individual Poster

LA-UR: LA-UR-18-26312

Efficient Algorithms for Stochastic Climate Adaptation Problem on Coastal Power Networks

In this project, we aim to develop efficient algorithms to solve a multi-period power system adaptation problem (i.e., bus hardening and expansion) that is scalable in the problem dimension and scenario size. The objective of this problem is to improve the resiliency of coastal power networks facing potential threats of sea level changes and storm surge events. In terms of the optimization model, the original problem is formulated as a two-stage joint chance-constrained problem with finite support and feasible mixed binary recourse. The problem is difficult to solve because it is a combination of stochastic programming and mixed integer programming. The only algorithm available is a scenario-based method with finite convergence and a global optimality guarantee, but the algorithm suffers from computational intractability when the number of scenarios is large. Compared with this work, we first reformulated the problem to avoid faulty decisions under extreme scenarios but provide scenario dominance relationships. Next, to speed up the algorithm, we developed techniques based on warm starts, tighter bounds on variables, and smart constraints. We also developed approaches based on model interpretation and related literature.

Student(s): Porter, Emily Samantha

Program: USG/Postbac

School: The University of Texas at Austin

PAD/Group: PADSTE/HPC-DES

Mentor: Baseman, Lissa, HPC-DES

Category: Computing

Type: Individual Poster

LA-UR: LA-UR-18-25756

Why Did the Model Cross the Road? : Comparing Automatic Generated Explanations of Random Forests

The prevalence of increasingly accurate, yet complicated, machine learning models in high-impact domains such as national security, finance, and social issues, continues to vastly outpace our ability to intuitively understand the reasons behind a statistical model's output. However, as these models are deployed to drive real-world decisions, the importance of being able understand and communicate reasons for a model's prediction becomes paramount. In this work, we compare a variety of current techniques for extracting human-understandable explanations for the predictions provided by a random forest classifier, one of the most commonly used statistical machine learning models. We consider both black-box and white-box explanatory techniques, including the recently popularized LIME (Local Interpretable Model-Agnostic Explanations), and a novel technique developed at Los Alamos National Laboratory which makes use of the internal structure of the random forest. As explainable machine learning is still a largely ill-defined field, we also discuss possibilities for quantitatively comparing automatically-generated explanations.

Student(s): Qiao, Zhi

Program: GRA

School: University of North Texas

PAD/Group: PADSTE/HPC-DES

Mentor: Chen, Hsing Bung, HPC-DES

Category: Computing

Type: Individual Poster

LA-UR: LA-UR-17-27639

Enhancing Storage Reliability via Declustered RAID

The reliability and availability of the storage system remains a challenge. Disk arrays (RAIDs) offer cost-effective improvement of throughput and redundancy, but prolonged rebuilt process after disk failure compromises system performance, reliability, and availability. Declustered RAID (dRAID) distribute data and parities evenly among disks in multiple arrays. It achieves maximum access parallelism and less-intrusive data reconstruction. In this project, we are evaluating the dRAID I/O and recovery performance in ZFS. The experiment variables include stripe widths, parity ratio, storage utilization rate, workload access pattern, redundancy level, etc. We benchmark and measure the storage I/O, throughput, random access performance, recovery time and speed, storage workload and wear during rebuilt. From the experiment results, we can observe that 1) dRAID evenly distribute the data, parity, and spare blocks. This permutation development based data organization ensures the even wear to the storage media and maximize the data access parallelism. 2) dRAID significantly speedup the disk array rebuilt time. The speedup is sub-linear to the number of disks contribute to the rebuilt process. And 3) Instead of using dedicated spare disk, dRAID use spare block that distributed among disk arrays. As a result, I/O performance benefit slightly from it compared with traditional software RAID in ZFS. We believe exascale storage system can take advantage of dRAID's excellent performance enhancement, to further improve the reliability and availability. However, there is one price to pay for such extraordinary speedup on disk array rebuilt: dRAID skips checksum scan and reconstruct data continuously, which might treat corrupted data as healthy one. We plan to solve this problem in our future work.

Student(s): Watson Ross, Chrys

Program: GRA

School: University of New Mexico

PAD/Group: PADSTE/NSEC

Mentor: Fairchild, Geoffrey, A-1

Category: Computing

Type: Individual Poster

LA-UR: LA-UR-18-26239

Troll Hunter: Understanding Swarm Behavior in Social Networks

Understanding the drivers leading to collective behavior is important for many areas in science from social movements and disaster response to Internet trolling. Abusive speech online, a form of Internet trolling, is a growing threat and can result in devastating consequences such as physical harm, manipulation, and control of public discourse. The ability to detect and track the spread of these behaviors is challenging given the vast amount of data and the variability in the text being used. In order to address this problem, we used reddit, a social news and media aggregation bulletin board type network. Using multiple machine and deep learning hate speech detection models and graph theoretical approaches, we analyzed titles and several sub-reddit threads. We inferred network structure, clustering, and dynamic characteristics of topics strongly correlated with abuse. These features will be applied to models to detect abusive speech, identify other topics that were missed by our language model, and predict troll swarm (brigading) events in near real-time.

Earth & Space Science

Student(s): Kintner, Jonas Andreas

Program:

School: Penn State University

PAD/Group: PADSTE/EES-17

Mentor: Cleveland, Mike, EES-17

Category: Earth & Space Science

Type: Individual Poster

LA-UR: LA-UR-18-26384

Low Yield Seismic Source Discrimination using Local and Regional Observation

Distinguishing between small tectonic and anthropogenic seismic sources remains as one of the challenges within the explosions monitoring community. Small seismic events necessitate the use of short period observations observed at local to near-regional distances, where a number of traditional seismic discrimination procedures have been shown to yield neither accurate nor precise results. We focus on exploiting a regional seismic dataset from events near the Bighorn Mountains, Wyoming. We experiment with a number of discrimination procedures to distinguish small ($ML < 4$) nearby earthquakes between 2000 and 2018, a collection of mining-related seismic events, and 21 single-charge contained chemical explosions associated with the 2010 Bighorn Arch Seismic Experiment (BASE). We test a number of measures that isolate different properties of waveforms generated by the three different source types. The results from this study show that the performance of particular discrimination procedures can be affected by path effects between source to receiver. We also find that the effectiveness of certain discrimination methods is influenced by the location of the source, particularly for signals generated by the BASE borehole explosions. This work shows that the implementation of different discrimination procedures allows us to effectively isolate unique characteristics between the source types, as well as identify the effects of near source material and propagation on discrimination performance.

Earth & Space Sciences

Student(s): Ahmmed, Bulbul

Program: GRA

School: Baylor University

PAD/Group: PADSTE/EES-16

Mentor: Viswanathan, Hari S, EES-16

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-25870

Finding productive zones in an unconventional reservoir using multi-frequency electrical impedance and flow model

Mapping the productive and non-productive zone in a horizontal well is critical for making informed decision about the hydrocarbon production. In this research work, we present an approach by combining information from multi-frequency electrical impedance tomography data (MFEIT) and flow data to find productive and unproductive zones around horizontal well. To this end, first, we perform a series of forward model simulations for various flow conditions using subsurface flow simulator PFLOTRAN to get hydrocarbon saturation. Second, we use this saturation profile in the Archie's law to obtain the electrical conductivities. Third, we use the E4D simulator with obtained electrical conductivities to simulate real and imaginary components of potential distribution in the reservoir. To test the proposed approach, we constructed a domain with dimensions of 1000×1000×1000 m³. The model had three zones of 200×100×200 m³ at several hundred meters depth from the surface. Two zones were assumed productive and other zone was assumed non-productive. Electrical conductivities of two orders of magnitude were explored to delineate productive and non-productive zones. Several hundred electrodes were used in multiple lines in E4D to simulate potential distribution and thousands of potential data were modeled. A total of 100 forward model runs are performed for an appropriate frequency range. Productive and non-productive zones showed indicative pattern of phase shift in voltage signals, which differentiate productive and non-productive zones.

Student(s): Behar, Hannah R

Program: USG/Postbac

School: Washington University in St. Louis

PAD/Group: PADSTE/EES-16

Mentor: Stauffer, Philip H, EES-16

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-25002

An Investigation of Plume Response to Soil Vapor Extraction and Hypothetical Drum Failure

Material Disposal Area L (MDA L) is an inactive waste site at Los Alamos National Laboratory. During site operation from the 1960s - 1986, waste drums were buried in the subsurface at MDA L. Subsequent drum leakage created a vapor plume of volatile organic compounds (VOCs) that is primarily located in the upper unsaturated Bandelier Tuff. However, there is concern that VOCs could migrate to underlying fractured basalt and ultimately reach the water table. Soil vapor extraction (SVE) was employed during 2015 to reduce plume mass, concentration, and extent. Then, extraction wells and boreholes were periodically monitored and sampled through 2017. In this study, the response of the plume to SVE is used to calibrate a three-dimensional numerical site model for MDA L. The model uses the porous flow simulator Finite Element Heat and Mass Transfer (FEHM) to simulate subsurface VOC behavior. Simulations include advection, diffusion, and plume interactions with topography. The site model is applied to simulations of VOC leakage in the event of hypothetical drum failure and potential SVE following the hypothetical drum failure. Results suggest that a small subset of boreholes could be monitored to provide detection of VOC releases, which could be effectively mitigated through SVE.

Student(s): Conley, Juliana Leigh

Program: USG/Postbac

School: University of Rochester

PAD/Group: PADSTE/EES-16

Mentor: Koo, Eunmo, EES-16

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26412

Turbulence in Wind Drives Variability in Wildland Fire Outcomes

In recent decades, wildland fire has become an increasing threat to life, health, property, and natural resources. The destructive and unpredictable nature of wildland fire makes it both critical to understand, and difficult to measure experimentally. Computational fire models help us make better generalizations about wildland fire behavior by allowing more controlled and replicable experiments. FIRETEC, the model used for this project, is a computational fluid model of coupled atmospheric/wildfire behavior. Each aspect of a FIRETEC simulation introduces variability into the final outcome. It is important to understand the dimension of variability that each aspect adds. Wildland fire behavior is known to exhibit sensitivity to wind conditions, particularly at the time of ignition. Turbulent wind fields are used in FIRETEC simulations, but the impact of variations in the wind field on variability of fire outcomes has not been quantified. To quantify this variability, we ran 27 simulations of fires in short grass that differed only in their spatial and temporal location within a larger turbulent wind simulation. To quantify impact on wildland fire behavior, we examine metrics of fuel consumption, rate of growth, and kinematic heat flux for each simulation. We find high variability between simulations, suggesting strong sensitivity of fire behavior to small perturbation in the wind field. Our results emphasize the need for ensemble simulations and highlight the predictive limitations of single fire simulations.

Student(s): Goldberg, Hannah

Program: USG/Postbac

School: Case Western Reserve University

PAD/Group: PADSTE/EES-17

Mentor: Syracuse, Ellen, EES-17

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26137

Determining the cause and nature of anomalous Rayleigh wave H/V ratio measurements in southern California

Seismic ambient noise cross correlation is becoming a popular tool in understanding the subsurface of the Earth. This method has been used to create more accurate seismic velocity models and can be used to better understand the structure at a range of depth, from the first tens of kilometers of the Earth's crust through the mantle. Rayleigh waves are the most easily observed seismic waves in cross correlation, and the recent use of the ratio of their horizontal to vertical amplitudes (H/V ratio) provides measurements that are very sensitive to shallow structure directly below seismic stations. Groundwater is one near surface feature that is of interest to seismologists and a nation that has experienced increased drought in recent decades. A current project at LANL is aiming to monitor temporal changes in the groundwater in southern California from the year 2000 through 2018 using Rayleigh wave H/V ratios, geodetic measurements, and GRACE gravity data. The Rayleigh wave H/V ratios are analyzed to the resolution of one week, but the measurements for several weeks are anomalous, showing much higher ratios across most stations. The goal of this project is to identify, within one hour's accuracy, when these anomalous measurements occurred, what caused them, and how to remove all the anomalous measurements in a systematic way. To this point, distant, high magnitude earthquakes have been found that coincide with anomalies' occurrences. Next, screening criteria will be determined to automatically remove time periods that likely contain signals from the earthquakes that cause these anomalies. Additionally, more sophisticated preprocessing techniques may be tested to prevent the anomalous measurements from appearing while retaining data from the affected time periods.

Student(s): Gorris, Morgan

Program: GRA

School: University of California, Irvine

PAD/Group: PADSTE/T-6

Mentor: Manore, Carrie Anna, T-6

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26117

Expanding a seasonal forecast of US West Nile virus for 21st century disease projections

West Nile virus (WNV) is the leading cause of mosquito-borne disease in the United States (US). Since its introduction to the US in 1999, the spatial distribution and number of WNV cases vary year to year. Transmission of WNV primarily occurs between birds, the main host, and mosquitos, the disease vector. Humans can contract WNV when bit by an infected mosquito. Previous studies showed that mosquitos and WNV cases are significantly influenced by environmental conditions including temperature, water availability, and humidity. Increased risk of WNV may follow after warm temperatures and mild winters, which may alter the distribution and abundance of the primary disease vector, the Culex mosquitoes, thus affecting the transmission of WNV. Other factors such as human demographics and the number of bird hosts can affect the risk of WNV, too. In this study, we built a statistical model to predict the number of WNV cases in each county using climate, county-level demographics, and bird survey data as predictors. Then, we used climate projections from Earth system models to determine if WNV will undergo a geographical shift in cases or a change in the number of cases in response to climate change. The ability of our model to assess changes in future WNV risk in response to climate change will be useful for public health officials in mitigating disease impacts.

Student(s): Graves, Emily Jo

Program: GRA

School: University of Texas at El Paso

PAD/Group: PADSTE/EES-17

Mentor: Rowe, Char, EES-17

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-25841

Investigating an Earthquake Sequence with Seismic Correlation and Array Methods

Using Montana Bureau of Mines and Geology and University of Utah earthquake locations and information for an energetic seismic sequence in Wyoming called the Jackson Swarm, we validate the catalog locations derived from multiple local and regional networks using reported P- and S- wave arrival times along with software and models similar to those originally employed. We then apply array processing methods to these events as recorded at the nearby Pinedale Seismic Array (PDAR) to the southeast, to address the question of location integrity in the absence of a well-distributed network. The Montana/Utah catalog provides only parametric data, not waveforms; however, we have continuous waveform data from PDAR for over two decades. During a visual inspection of PDAR data extracted for the catalog events, we observed additional, unreported events, which is to be expected during an energetic swarm or seismic sequence. The casual observation of missed events strongly implies that more such missed events can be found in the data, which could improve the completeness of the earthquake catalog for the Jackson, Wyoming area. Catalog completeness improves our assessment of a region's tectonic behavior and earthquake exposure. To look for recurring swarm or earthquake sequence behavior, we apply waveform correlation methods to scan two decades of continuous PDAR waveforms, comparing to several "template" events selected from the Jackson Swarm catalog, to identify repeating events from the source area of the swarm.

Student(s): Miller, Greta Amy

Program: USG/Postbac

School: Princeton University

PAD/Group: PADSTE/EES-16

Mentor: Bennett, Katrina Eleanor, EES-16

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: 'LA-UR-18-26413

Climate Change Impacts on Water in Northern New Mexico

This project will focus on a study examining the impacts of climate change in Northern New Mexico, including impacts to vegetation, soils, and infiltration. The student's primary tasks will focus on data collection, management, and visualization for a range of 'Big Data' analytics and geospatial information including vegetation coverage, soils, geology, and model results, and non-spatial information including stream gage data. The student will also help to set up ecohydrological models, which will potential include the USGS INFIL model and the ParFlow-CLM hydrological model. Key outputs will include a geodatabase for the Pajarito Plateau, ecohydrologic model output, and a presentation describing the major goals and outcomes of the work. The work will focus on open and publishable science.

Student(s): Rosa, Kevin Lynch

Program: GRA

School: University of Rhode Island

PAD/Group: PADSTE/NSEC

Mentor: Petersen, Mark Roger, CCS-2

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26017

Variable-resolution ocean model improves physics at reduced computational cost

Climate models need finer resolution in order to resolve important physics which are currently added in as parameterizations. Ocean measurements show highly energetic localized regions where processes down to the scale of 6-10 km play an important role in the climate system. Previous climate models have employed rectangular grids which produce nearly-uniform grid resolution globally and require lots of grid cells to resolve finer scales. A new modeling system, the Model for Prediction Across Scales (MPAS), aims to solve this problem by employing an unstructured mesh where resolution (and therefore computing resources) can be focused on specific regions of physical significance. In the present study, we employ MPAS-Ocean with refined resolution in the Southern Ocean and show that the variable-resolution model can produce similar Southern Ocean results as a global high-resolution model but at a greatly reduced computational cost. This finding motivates the future application of this grid-refinement approach to additional key regions such as the Gulf Stream and coastal upwelling zones. Although the computational resources required to simulate the climate at global high-resolution may be over a decade away, we can exploit the ocean's non-uniform distribution of kinetic energy in order to focus our resources on the regions where fine-scale processes have the largest effect on the climate system.

Student(s): Sare, Robert Martin

Program: GRA

School: Stanford University

PAD/Group: PADSTE/EES-14

Mentor: Rowland, Joel C, EES-14

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26273

Fluvial response to land use change measured in Landsat time series of migrating rivers

River geometry is sensitive to many factors, including discharge, bank materials and cover, and the caliber and quantity of sediment supplied to the channel. This project aims to measure river migration rates over decadal time scales at sites experiencing significant upstream land use change. Case studies for potential human-induced fluvial change include the watershed of the Rio Madre de Dios of Peru, where gold mining has stripped the landscape of vegetative cover and serves as a significant source of river sediment, and the Mamoré River in Bolivia and Brazil, where agricultural development near a tributary has led to diversion of water into manmade irrigation channels. These and other major rivers are imaged by satellites of the Landsat program, which provides moderate resolution optical and infrared imagery from 1972 to present. We explore methods for segmentation of satellite images to extract the extent of active river channels, a key component of a pipeline for measuring active channel width and bank erosion and accretion rates. This workflow is applied to imagery from 1984 to present to quantify the effect of land use changes on migration rates. The accuracy and common success and failure modes of various segmentation methods will be discussed in terms of their impact on migration rate estimates. Python utilities for image segmentation and generating training and validation datasets from satellite imagery using Google Earth Engine and cloud resources will be presented. Methods developed in this project will further studies of river migration worldwide. These measurements can provide important constraints on Earth system fluxes where soil organic carbon may be released by increased erosion, and they may document local fluvial response to human activity and extreme events, as well as larger-scale impacts of climate change.

Student(s): Sherman, Thomas James

Program: GRA

School: University of Notre Dame

PAD/Group: PADSTE/T-CNLS

Mentor: Hyman, Jeffrey De'Haven, EES-16

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-25368

Characterizing the impact of particle behavior at fracture intersections in three-dimensional fracture networks

When particles enter a fracture intersections within a discrete fracture network (DFN) how they should behave depends upon the local Peclet number (a dimensionless ratio of advective and diffusive forces) within the intersection. However, the actual fluid dynamics along the intersection are a sub-grid scale process in DFN modeling that is not explicitly resolved. This complex system along fracture intersections requires detailed analysis and a robust modeling approach to properly upscale the physical phenomenon. Currently, there are two generalized rules to which particles can adhere. There is complete mixing (where diffusion is dominant and particles can jump pathlines) and streamline routing (where particles adhere to their respective pathlines). Our DFN models, both the high-fidelity and graph-based models, only consider complete mixing. However, this is unphysical for many systems of interest, e.g., low yield clandestine nuclear testing and containment remediation. We implement streamline routing in our high-fidelity DFN model. Comparison of the mixing rules in the two systems is quantified by considering solute transport behavior, e.g., breakthrough times and dispersion, along with appropriate uncertainty quantification to properly characterize the impact of adopting particular mixing rules at fracture intersections in three-dimensional fracture network.

Student(s): Sockwell, Kenneth C

Program: Post Masters

School: Florida State University

PAD/Group: PADSTE/T-3

Mentor: Van Roekel, Luke, T-3

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-25865

Exponential Integrator - Krylov Methods For Mimetic Ocean Models

Climate modeling is a computationally intense endeavor which requires multi-resolution and multi-physics methods to faithfully and accurately simulate world climate over long time spans. Recently, the DOE Office of Science has initiated the Energy Exascale Earth System Model (E3SM), which contains the Model for Prediction Across Scales-Ocean (MPAS-O), the model responsible for the ocean. The MPAS-O software aims to accurately capture the highly disparate, multiple scales occurring in ocean modeling by using highly nonuniform spatial meshes. Currently, there is a gap between highly nonuniform spatial schemes and the time-stepping schemes needed to complement them, especially with regard to the resulting CFL time-step restriction. Exponential integrators (EI) in combination with rational Krylov methods can supersede the CFL restricted time-step with a larger time-step while still attaining stability. EI methods in combination with rational Krylov methods give rise to a time integrator that is truly independent of the CFL. However, these methods require costly matrix inversions in the EI method as opposed to matrix-vector multiplications done in normal Krylov methods. In order to make this methods efficient, methods which mitigate or minimize the cost of the matrix inversion are a high priority.

Student(s): Trejo-Lorenzo, Imelda

Program: GRA

School: The University of Texas at Arlington

PAD/Group: PADSTE/EES-16

Mentor: Viswanathan, Hari S, EES-16

Category: Earth & Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-25968

Uncertainty Quantification and Machine Learning Methods in the Graph Transport Model

Graph transport model is a novel approach to simulate flow and transport of solutes along discrete fracture networks. The model efficiently calculates the travel times of the transported particles from an inflow to an outflow position. However, its accuracy decreases as the number of fractures in the network increases. In this work, uncertainty quantification is performed to identify and quantify the model input uncertainties. Sensitivity analysis is calculated on the quantity of interest of the model called breakthrough curve which is the probability distribution function generated by the exit time of the transported particles. Then, machine learning methods are used to classify and predict breakthrough curves from different discrete fracture networks.

Earth and Space Sciences

Student(s): Bailey, Connor

Program: USG/Postbac

School: University of California, Davis

PAD/Group: PADSTE/MPA-MAG

Mentor: Singleton, John, MPA-MAG

Category: Earth and Space Sciences

Type: Individual Poster

LA-UR: LA-UR-18-26062

On the information carried by electromagnetic radiation launched from accelerated polarization currents

In the past 15 years, there has been renewed interest in the emission of radiation by polarization currents that travel faster than the speed of light in vacuo. Such polarization currents are produced either by photoemission from a surface excited by an obliquely incident, high-power laser pulse, or by the application of carefully timed voltages to multiple electrodes on either side of a slab of a dielectric such as alumina; the latter method has been developed mainly at LANL, and is more convenient for laboratory experiments and future technological development. This poster considers the information conveyed in the signals broadcast by such polarization currents when they are accelerated. Using both numerical simulations and radiofrequency experiments, it is found that a time-dependent amplitude modulation imposed on the polarization current is reproduced exactly in the received signal only when the detecting antenna is close to a particular point, the position of which is related to details of the acceleration. At other points, the signal is scrambled. The result has implications for possible methods of secure communication and for astronomical observations of objects such as pulsars.

Engineering

Student(s): Adams, Matthew James

Program: GRA

School: Arizona State University

PAD/Group: PADSTE/NSEC

Mentor: Mascarenas, David Dennis Lee, NSEC

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25855

High speed ESPI for structural health monitoring via full-field vibrational displacement measurements

The modal vibrations of a structure are characteristic of that structure's physical properties. For instance, a metal plate with corrosion will exhibit different vibration modes than one without corrosion. Non-destructive modal vibration testing provides a way to identify whether or not a structure exhibits damage. Existing full-field displacement measurement techniques (direct strain imaging and digital image correlation) track dots on the surface of a structure to measure surface displacement. Electronic speckle pattern interferometry (ESPI) uses a laser to form fringe patterns caused by induced microscopic displacements of the structure, removing the need to prepare the surface. This work confirms the use of ESPI to measure full-field surface vibrational displacements. We then used the measured displacements to calculate differences in modal vibrations from structures with varying types of damage. Future work will investigate direct inverse characterization of structures from ESPI vibrational displacement measurements.

Student(s): Bhela, Siddharth

Program: GRA

School: Virginia Tech

PAD/Group: PADSTE/T-5

Mentor: Nagarajan, Harsha, T-5

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26447

Optimal Topology Design for Disturbance Minimization in Power Grids

The transient response of power grids (modeled as networked linear dynamical system) to external disturbances influences their stable operation. To this end, different controllers and dampers are placed in networks to minimize the probability of catastrophic failures due to such disturbances. In recent years, due to reduction the total number of large inertial devices in the network (which absorb disturbances), the ability of the network to withstand big disturbances have gone down. In this setting, researchers have focused on new controller design as well as optimal operation, placement, and communication between existing devices to maximize their capacity in disturbance reduction. This project, plans to understand topology-design, communication-design and placement policies in low inertial micro-grids and transmission grids to attain desired control goals. Using a control theoretic framework the optimization problems will be formulated as mixed-integer combinatorial problems

Student(s): Brand, Howard James; Kauppila, Tia Morgaine; Wielgus, Kayla Marie

Program: USG/Postbac

School: Michigan Technological University

PAD/Group: PADSTE/NSEC

Mentor: Mascarenas, David Dennis Lee, NSEC

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25856

Imager-based Characterization of Viscoelastic Material Properties

In this work we explore the use of emerging full-field, high-resolution, modal identification techniques from video to characterize viscoelastic material properties. Currently, there are no cost-effective methods to directly measure viscoelastic material properties at intermediate strain rates. These properties can be measured at low strain rates using quasi-static loading techniques, while Split-Hopkinson's bar tests are used at high strain rates. Determining material properties at the intermediate strain rate regime is challenging as it requires large, expensive testing apparatuses and involves complex experimental protocols. An imager-based technique would provide a simpler, more affordable method for measuring viscoelastic material properties at these strain rates. To obtain measurements for intermediate strain rates of viscoelastic materials, we develop a testing protocol that involves creating a simple structure from the material-under-test and measuring its vibrational response using an imager. A finite-element model of the viscoelastic testing structure is also constructed. We extract full-field, high resolution modal shapes and coordinates from the video measurements of the structure's vibrations in the desired strain regime. The frequencies of oscillation and the damping ratios are then identified. This information is used to perform model updating on the viscoelastic material properties of the finite-element model, resulting in an improved estimate of these properties. Imager-based techniques are attractive for explosive testing applications because the optics can be adapted to address the small sample sizes necessary for explosive testing. In addition to advancing viscoelastic material modeling, this work points toward the development of an imager-based modal analysis technique for identifying the structural dynamics of micro-scale structures. At this small scale, conventional contact-based sensors would result in mass-loading effects, yielding inaccurate measurements. As a solution, our full-field, high-resolution imager-based technique provides a method to characterize viscoelastic material properties while also demonstrating potential for future work in identifying structural dynamics of micro-scale structures.

Student(s): Figueroa, Alejandro Luis

Program: GRA

School: Purdue University

PAD/Group: PADSTE/AET-6

Mentor: Espy, Michelle A, AET-6

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26238

Density measurements using Computed

X-ray CT allows for the internal composition, density, and structure of a sample to be analyzed without damaging the sample itself. This knowledge can be used to create a better understanding of the behavior of a sample in destructive testing. This is of particular interest to high explosives where a formal understanding of the relationship of the structure and density to behavior is not fully known. Specifically, density variations within a material can influence the performance, but the classical method of immersion density measurements provides only a coarse sampling and is destructive. By analyzing the X-ray attenuation of the varying densities and comparing it to immersion density data a non-destructive method to calculate the density of a HE sample using X-Ray CT can be established. This will help create a link between density and the behavior in HE samples.

Student(s): Horan, Caleb Josef

Program: High School

School: Colorado State University

PAD/Group: PADSTE/SIGMA-2

Mentor: Carpenter, John S, SIGMA-2

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26038

A New Phase of Development in the Diagnostic Capabilities of Additive Manufacturing

Presently, the process of finding defects within an additively manufactured part is high cost, time consuming, and incapable of characterizing pores during fabrication. Instead, a pyrometer system called “Therma-Viz” collects data which can be processed to determine the likelihood of defects in the part based off of melt pool characteristics. This project has three goals. The first goal is to improve the accuracy of this defect detection process by testing different diagnostic parameters with relation to melt pool characteristics. An analysis function will be created to quantify the defect detection effectiveness by statistically comparing the uniqueness of frames known to contain defects. This function will be applied to the outputs of the processing script over an experimental matrix of input parameters for the purposes of optimization and process parameter sensitivity. Second, in this study, inefficiencies will be identified and corrected in the Python script. The present script is constructed for scientific exploration but could be optimized once critical outputs are identified. Third, this study will compare pre-written blur functions that are used to realistically curve data for efficiency and applicability between several coding languages. The impact of this study will be a more effective and efficient diagnostic tool.

Student(s): Hypes, Victoria D

Program: USG/Postbac

School: New Mexico Tech

PAD/Group: PADSTE/C-CDE

Mentor: Hollis, William Kirk, C-CDE

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25652

Modeling Tritium Fuel Cycling and the Impact of Liquid Metal Plasma Facing Components for Fusion Energy

Fusion power reactors have been under design for over 50 years as an option to address world and US power demands. The tritium fuel cycle is an integral part of any reactor design. Tritium inventory in each individual component of a fusion fuel cycle affects lifetime performance, output and safety of the overall system. Every reactor component has its own inventory cycle, and the success of the whole depends on the operational performance and inventory of the individual parts. Each component will depend on input from another part of the reactor, making modeling complicated. First order differential equations have been commonly used to assess the system, but have not been sufficiently accurate to predict the fueling cycle. Parametric analyses are being assayed to give a more accurate accounting and better understand the interactions of these systems and will be presented. Adding to this complex analysis is the addition of liquid metal on the plasma facing components to improve lifetime performance of the reactor. Current work has been conducted to understand the impact of this type of wall on the tritium fuel cycle for the DOE Fusion Nuclear Science Facility (FNSF) design. Particularly important is the interaction of tritium with a thin layer of liquid metal protecting the reactor wall. Several liquid metals are under consideration, and analysis of tritium retention and recycle must be done for each. This poster will present the analytic foundation of the tritium recycle rate, as well as a review of the modeling methods currently in place.

Student(s): Irish, Laken S

Program: USG/Postbac

School: Arizona State University

PAD/Group: PADSTE/AET-1

Mentor: Ouellette, Brittany Joy, AET-1

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25527

Distributed Fiber Optic Sensing

Optical fibers are being explored as a means to detect strain and temperature differentials in components when exposed to various loads and thermal conditions, respectively. Fibers embedded within or adhered to the surface of a part can capture fine resolution data specific to a precise location on the part. Strain may be measured along the entire length of the fiber by collecting Rayleigh backscattered light, the backwards radiation of incident light from particles much smaller than the incident wavelength. A small amount of Rayleigh backscatter is measurable in fiber optics due to the microscopic variations in the fiber's core density and refractive index. Wavelength data may be taken at a minimal gage spacing of 0.65 mm, providing over 1,000 data points per meter of fiber. The unstrained baseline wavelength data is cross correlated with the strained wavelength data, then converted to strain using an empirically determined calibration coefficient. The purpose of this project is to verify the effectiveness of optical fibers as strain sensors. This will be demonstrated with LUNA's ODISI 6104 sensing system by testing a simple additive manufactured (AM) part geometry with an applied axial loading condition. The strain data will be compared to other developed, reliable methods including Finite Element Analysis (FEA) with ANSYS, Digital Image Correlation (DIC) measurements, and analytical calculations. Load path analysis and point strain are two specific metrics that will be analyzed. If proven effective, LUNA's ODISI 6104 system will be used for further research on AM parts, with key focus areas describing the change in material properties with varying print settings, understanding the material behavior of the inner layers of a printed part, and demonstrating the great potential of embedding distributed sensing in AM components.

Student(s): Lam, Jared Tate

Program: USG/Postbac

School: New Mexico Institute of Mining and Technology

PAD/Group: PADSTE/EES-14

Mentor: Dubey, Manvendra Krishna, EES-14

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26474

A Novel Humidity-Controlled System for Measuring Enhanced Light Absorption by Water-Coated Soot

Aerosols affect the Earth's radiation balance by absorbing or scattering radiation resulting in either a warming or cooling effect, respectively, in the atmosphere. The transition depends on surface albedo as well as aerosol single scattering albedo (SSA) which quantifies the brightness of the aerosol. SSA depends on aerosol chemical properties including its hygroscopicity which quantifies aerosol water uptake as a function of relative humidity (RH). Once a particle reaches deliquescence humidity, the size of the particle significantly increases as it forms a water droplet. This affects aerosol optical properties by altering the chemistry, size, and/or morphology of the particle. Many climate model simulations demonstrate that water coatings on soot particles absorb more sunlight, amplifying their warming effect, though this effect has not yet been measured. In order to probe these key RH dependence effects, we have developed a novel system that uses a Cavity Attenuated Phase Shift instrument to simultaneously measure aerosol light scattering and extinction (where light extinction is the sum of light scattering and absorption) under humidified conditions (RH>70%) and dried conditions (RH<20%) at 450nm. An actuated ball valve that alternates between humidified and dried sample lines makes it possible to observe changes in optical properties with an equilibration time of less than 30 seconds. Via LabVIEW, the humidifier may be controlled to attain target RH on a selectable path-switching frequency (e.g. 3 minutes). Change in optical properties is quantified as $f(RH)$ which is equal to the ratio of light scattered under humidified conditions to light scattered under dried conditions, and this ratio may be applied to light scattering, extinction, or absorption. Our goal is to report the first direct observations of water coating enhancements of soot's light absorption by lensing in the

Student(s): Li, Wenting

Program: GRA

School: Rensselaer Polytechnic Institute (RPI)

PAD/Group: PADSTE/T-CNLS

Mentor: Chertkov, Michael, T-4

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26423

Real-time Faults Location Through Deep Learning Classifier

Locating faults in power grid efficiently is pivot to improve the system stability and reliability. Most operations after faults are automatically taken according to the status of circuit breakers or other devices, but many mis-operations have been reported to cause the power system collapse. Artificial intelligence (AI) methods are proposed to locate faults through the data obtained by phasor measurements unit (PMU) of multiple buses, but the existing algorithms often require high sampling rate, complicated models with low physical interpretations, complete observability, and mostly are

Student(s): Liao, Ashlee Shiueh Ni

Program: USG/Postbac

School: North Carolina State University

PAD/Group: PADSTE/NSEC

Mentor: Mascarenas, David Dennis Lee, NSEC

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26207

Combined novel application of a silicon retina and stereo imagers with machine learning techniques to infer depth

The indoor environment often presents many barriers that can be challenging for aerial robots to navigate at high velocities due to varying lighting and environmental conditions. Aerial robots can be deployed to rapidly gather information about a region, which has applications in disaster response and infrastructure inspection. For successful high-speed navigation, a lightweight, low-power, sensor that can capture data at an effective frame rate (based on the velocity of navigation) and estimate depth information is necessary. The proposed mechanism is the combination of a silicon retina imager that infers depth based on a machine learning algorithm. The silicon retina imager is a low-power device that asynchronously captures event information due to temporal changes in a monocular image. Therefore, it only captures data when intensity changes occur, enabling the silicon retina to rapidly obtain data faster than conventional imagers of comparable sizes at a lower bandwidth. The event data can be used to infer the depth of the environment relative to the imager by using a machine learning algorithm that is taught on a dataset of stereo images. The stereo images provide the ground truth for depth by mimicking the methods used in vertebrate binocular vision, which estimate depth by utilizing the disparity of the pixels between the left and right images. By combining the silicon retina and stereo imagers with machine learning, an effective, low-power navigation sensor can be developed for a high-speed, high-performance aerial robot.

Student(s): Martinez, Alejandro Sebastian

Program: USG/Postbac

School: University of New Mexico

PAD/Group: PADSTE/AOT-IC

Mentor: Shelley Jr., Fred, AOT-IC

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26402

LANSCE-Alarm Detection Device

The Occupational Safety and Health Academy (OSHA) clearly specifies that the essential purpose of any alarm system for employees is to reduce accidents and injuries. In order for this goal to be achieved, alarm systems need to function properly and procedures should be established to clearly alert employees to emergencies in the workplace. Within the LANSCE facility, there are numerous existing alarm systems created to detect fire, neutron leaks, and radiation. Since every alarm typically has a different response, it can become confusing for employees on how to respond. The intent of the development of the alarm detection device that I'm working on is to minimize confusion for employees. Additionally, the device needs to be easily heard within the workplace. The approach I've taken will hopefully achieve this by creating a device that detects decibels emitted when the alarm goes off, in turn activating an audio file that is played on a speaker. The activated audio file will instruct workers what to do. This alarm detection device is completely separate and would not interfere with any other alarms currently in operation.

Student(s): Peck, William Jordan

Program: GRA

School: The Pennsylvania State University

PAD/Group: PADSTE/AET-2

Mentor: Moulton, Travis, AET-2

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26237

Economic Order Quantity for Drum Purchasing

Within classical production modeling, economic order quantity is a necessary model that calculates a feasible order quantity as well as a feasible reorder period. The focus of this paper is applying the economic order quantity model to container kit assembly production at TA-22. Statistical tests, such as the Kolmogorov – Smirnov Goodness of Fit Test are employed to estimate annual demand. Multiple holding costs are presented, each representing the cost to store ordered material in different buildings. All manufacturing process experience a degree of uncertainty, either in processing times or future demand, this forces the process to tolerate a certain degree of risk. Presented within are multiple scenarios that assume different levels of risk. While a specific scenario is prescribed by the author, the underlying concept pertaining to the relationship of risk and its impact on inventory level is thoroughly examined so as to provide process experts with an understanding regarding the implications of risk on the process. The result is a recommendation that suggests values for order quantity and reorder period, as well as a risk tolerance level that aims to balance drum inventory levels and the probability of demand exceeding supply and creating a stock out.

Student(s): Purcell, Dylan Chance

Program: USG/Postbac

School: New Mexico Institute of Mining and Technology

PAD/Group: PADSTE/P-21

Mentor: Nath, Pulak, P-21

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26210

Fully Automated Serial Dilution Using Integrated Magnetically-Coupled Micro-valve Arrays

Operations that can be performed in the laboratory beforehand, such as serial dilution to prepare a reagent or sample, are often left out of the microfluidic device due to the complexity of integration. We demonstrate a microfluidic serial dilution system that relies on integrated, magnetically-coupled arrays of valves operated by a single driver unit. The system is composed of a microfluidic card, a magnetically-coupled driver disc, and a peristaltic pump. Internal magnets, which act as valves within the microfluidic card, are actuated vertically by the magnets within the driver. The driver is designed in such a way that by rotating it to specific positions, specific set of valves can be opened or closed. This method can provides several benefits including, • Automation: The process was automated by using a Raspberry Pi. The automated platform can be programmed to perform serial dilution with any given target concentration, reducing human error and loss associated with pipetting. • Reduced Peripherals: The sequence of mixing for serial dilution can be carried out using a single stepper motor taking up minimal space while also opening the potential for operation outside of laboratory settings. • Versatile integration into Lab on a chip platforms: By controlling the flow rates and timing of the valve switching, it is possible to design serial dilution with any incremental dilution ratio without changing the microfluidic channel dimension. The microfluidic card and the driver disc were fabricated using a laser based micro-patterning and lamination of polymer film/sheet. This work will present the challenges and potential of the serial dilution platforms for applications in lab on a chip and demonstrate our approach to using an array of magnetically coupled micro-valves to perform fully automated serial dilution.

Student(s): Riback, James

Program: USG/Postbac

School: UC San Diego

PAD/Group: PADSTE/NSEC

Mentor: Mascarenas, David Dennis Lee, NSEC

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-25858

Augmented Reality for Post-Earthquake Inspection

Following a form of natural disaster, such as an earthquake in California, engineers are dispersed to conduct rapid condition assessment and conduct structural health monitoring on structures in the affected area. The tools available to inspectors to perform their evaluations have been limited to a pen and paper to fill out data collection forms. In this work we explore improving this process with Augmented Reality (AR), by equipping inspectors with a new tool to collect, interact with, and analyze inspection data. A primary goal is to integrate automatic corrosion/crack damage detection into Augmented Reality. A previous entropy algorithm was tested on a RGB Camera displaying gradient magnitudes and highlighting cracks in concrete. We plan to deploy this algorithm to the AR Headset, allowing engineers to automatically locate and tag possible seismic damage on-the-fly. Instead of having to pre-review field data and sketching building files, the AR Headset comes equipped with a depth imager. This imager can be used to make 3D models of critical infrastructure in real time during an inspection. These existing holograms could bring up previous data such as age, size, construction type, and any preceding irregularities. The use of AR also provides an enhanced form of communication between different inspectors. Instead of having to post paper warnings around the affected structure, AR allows us to superimpose holographic data pins onto the real world. This will warn future inspectors who come by the area that the following structure has been inspected, and will notify if the structure contains any safety concerns. Overall, AR is a promising tool for enhanced post-earthquake infrastructure inspection, mapping buildings on site, generating models, and providing consistency between inspectors. This technology could provide increased speed and quality to post-earthquake inspections and result in a development towards more accurate and safe structure determinations.

Student(s): Ruiz, Javier Matias

Program: GRA

School: University of California, San Diego

PAD/Group: PADSTE/AET-5

Mentor: Harden, Troy Anthony, AET-5

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26386

Dynamic Path Planning for Robotic Manipulators

Robotic manipulators are often used in industrial applications such as the handling and assembling of materials. In cases where we might want a manipulator to assist a human in constrained environments, such as a glovebox, the manipulator needs to be able to handle navigating through an environment which could be changing due to human action. This project modifies an existing path-planning algorithm based on an optimal rapidly-exploring random tree. The existing algorithm adapts the tree to take into account changing obstacles in the workspace. The modification of the algorithm allows for the path-planner to also track a moving target without having to re-plan from scratch whenever the target is moved. The new algorithm is tested on a simulation of a robotic manipulator.

Student(s): Schultz, Aubrey Lynn

Program: USG/Postbac

School: Oklahoma State University

PAD/Group: PADSTE/AET-2

Mentor: Stevens, Garrison, AET-2

Category: Engineering

Type: Individual Poster

LA-UR: LA-UR-18-26287

Simulating Shipping and Receiving Changes in Plutonium Facility

The plutonium facility at Los Alamos National Laboratory (PF-4) is planning for a change from existing FL nuclear shipping containers to new MD-2 containers. Transition to shipping and receiving of the new containers requires analysis of potential modifications to facility equipment and worker crews. In particular, the significantly increased weight of MD-2 containers requires integration of additional cranes to support the receiving and shipping processes. The receiving process for MD-2 containers is evaluated by a discrete event model using ExtendSim simulation software. The model is leveraged for preliminary analysis of the process flowsheet as well as optimization of resources. Initial analysis calls to attention potential bottlenecks in the process and presents solutions for future consideration. Results of this study seek to guide facility management towards the best scenario for a quick and efficient transition plan prior to MD-2 implementation.

Materials Science

Student(s): Barrett, Timothy James

Program: GRA

School: University of New Hampshire

PAD/Group: PADSTE/MST-8

Mentor: Mccabe, Rod, MST-8

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26301

Texture Interpolation: Application to Formed Depleted Alpha-Uranium

Metal components produced by processes such as forming and drawing exhibit spatial variations of properties and underlying microstructure. Microstructure evolution based finite element models, used to accurately predict the performance of these components, require microstructure (texture) input at each integration point, and experimental textures are measured only for limited number of positions. Here we develop a generalized spherical harmonics (GSH) based texture interpolation/regression scheme to enable microstructure evolution based finite element crystal mechanics-based simulations. We demonstrate the scheme using formed uranium hemispheres. Neutron diffraction is used to measure textures at discrete latitudes (every 10° from pole to equator) and longitudes (every 15° degrees between 0° and 180°) about the part, and these experimental textures vary considerably with position. We use texture interpolation to enable the elastoplastic self-consistent (EPSC) polycrystal model within Abaqus finite element to simulate the spatial and temperature dependent behavior of a formed uranium hemisphere. Thermal expansion and elastic stiffness components are predicted to vary by 67% and 15% from pole to equator, respectively, and considerable distortion is predicted upon heating.

Student(s): Birnbaum, Serena M

Program: USG/Postbac

School: Case Western Reserve University

PAD/Group: PADSTE/MPA-MAG

Mentor: Singleton, John, MPA-MAG

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-25790

The de Haas-van Alphen effect in AuBe, a non-centrosymmetric superconductor

Noncentrosymmetric superconductors, such as AuBe, are a hot topic in Condensed Matter Physics; they lack spatial inversion symmetry, leading to exotic properties in their superconducting state. My work involves searching for unusual features of the electronic bandstructure of AuBe in its normal metallic state, the precursor to superconductivity. In this way, some strange features of the superconductivity of AuBe, such as its anomalously high upper critical field, might be understood. The electronic bands of materials like AuBe are usually measured using the de Haas-van Alphen effect, oscillations of the magnetization that are periodic in $1/(\text{magnetic field})$. Each series of oscillations corresponds to an extremal orbit around the Fermi surface, the surface of constant energy in k-space (momentum space) that represents the filled electronic bands of the metal. By measuring the oscillations for many orientations of the magnetic field with respect to the crystal axes, the three-dimensional shape of the Fermi surface may be mapped out. Hence, a single crystal is usually required for such experiments. Unfortunately, single crystals of AuBe have proved impossible to grow thus far; the best material is polycrystalline, i.e., made up of many tiny crystals at random orientations. Nevertheless, ingots of AuBe show a plethora of de Haas-van Alphen oscillations at temperatures in the range 0.5 to 20 K and in pulsed magnetic fields of up to 60 T. By using a Fourier-transform program that gives both amplitude and phase information, and by novel and careful analysis of the field- and temperature dependence of the oscillations, it has been possible to map four sections of the Fermi surface of AuBe in detail and confirm a preliminary model of its electronic bandstructure. Interestingly, one of the bands is Dirac-like; the electrons in it behave like hyper-relativistic particles, with energies that are directly proportional to their momenta.

Student(s): Edgar, Alexander Steven

Program: GRA

School: University of Oregon

PAD/Group: PADSTE/MST-7

Mentor: Yang, Dali, MST-7

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-25242

Transition characterization of poly(ester urethane) elastomer via thermal and mechanical analyses

A systematic series of experiments is presented utilizing Thermogravimetric Analysis (TGA) to establish degradative limits of Estane®5703 poly(ester urethane) block copolymer elastomer. Subsequently, Modulated Differential Scanning Calorimetry (MDSC) is used to resolve the overlapping melt peaks found when analyzing Estane. Additionally, Dynamic Mechanical Analysis (DMA) is used to verify the melt temperature by thermal step-wise, creep analysis extrapolating temperature dependent moduli to zero. In all experimental sets, method parameters are optimized through diagnostic procedures, leading to method parameters tailored to the polymer. Along with MDSC and DMA method development, material thermal properties will be discussed. This work was supported by the US Department of Energy through the Los Alamos National Laboratory Enhanced Surveillance Program.

Student(s): Farnin, Christopher Joseph

Program: USG/Postbac

School: Lehigh University

PAD/Group: PADSTE/SIGMA-DO

Mentor: Montgomery, Colt James, SIGMA-1

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26208

Effects of Non-Contact Supports on Laser Powder Bed Fusion Parts

Non-contact supports (NCS), support structures printed alongside a powder bed fusion additively manufactured (AM) part, will be investigated as a method of regulating the cooling rate of a metal part as it is printed. The objective of this project is to observe the effects of NCS on the grain size, phases and pores formed, and surface finish when placed at varying distances from a printed sample. The hypotheses are that NCS closer to the sample block will result in smaller grains, a higher volume fraction of nonequilibrium phases, a rougher surface finish, and an increase in keyhole porosity. To test these hypotheses, an EOS M290 printer, using 304L stainless steel powder, will be used to print rectangular samples with four NCS at distances of 150, 225, 300, and 375 μm away. After processing, the surface roughness of the sample block will be measured using laser profilometry. The sample blocks will be cut, metallographically prepared and analyzed under a LOM to determine the average grain size, and volume fractions of the phases formed. Trends between these measured parameters and the NCS distances from the sample block will be noted and analyzed.

Student(s): Flanagan, Rachel Marie

Program: GRA

School: University of California, San Diego

PAD/Group: PADSTE/MST-8

Mentor: Fensin, Saryu Jindal, MST-8

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26126

NON-EQUILIBRIUM MOLECULAR DYNAMICS SIMULATIONS OF EJECTA FORMATION IN HELIUM-IMPLANTED COPPER

The shock behavior of helium-implanted copper single crystals is investigated using non-equilibrium molecular dynamics simulations. Although copper has been well-studied by both experiments and simulations, its dynamic behavior containing heterogeneities such as helium continues to be of great interest to the materials science community. We specifically explore the production of ejecta, which is formed when a planar shock wave reaches a free surface. Both atomic helium and helium bubbles are randomly generated and implanted in a perfect fcc copper single crystal. The crystal is then shocked along the [111] direction using a controlled piston. We present results describing the dependence of ejected mass on the shock strength, as well as the size and velocity distributions of the ejected mass.

Student(s): Hamblin, Ryan Lyle

Program: USG/Postbac

School: University of New Mexico

PAD/Group: PADSTE/MPA-CINT

Mentor: Ivanov, Sergei A, MPA-CINT

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26449

Using Biophysical Techniques to Interrogate Soft Matter Nanoscale Structures

Soft materials are easily deformable under energies equivalent to thermal energies at room temperature. Characterizing soft matter structures presents unique challenges, due to the ease of deforming or destroying such structures with commonly used characterization techniques. These difficulties are compounded when dealing with structures at the nanoscale, well past the diffraction limit for optical microscopy. This project focuses on employing techniques used to characterize such soft matter nanoscale structures. We study pS-pEG and pBD-pAA, two amphiphilic block copolymers that can self-assemble into higher-order structures in aqueous solution. Such structures are of interest for their biomimetic properties, making them promising for targeted drug delivery. To characterize pBD-pAA and pS-pEG nanostructures, we combine dynamic light scattering (DLS), atomic force microscopy (AFM), and transmission electron microscopy (TEM). A new methodology employing Förster Resonance Energy Transfer (FRET) to pBD-pAA micelles was also developed, which our ongoing work seeks to improve.

Student(s): Huang, Sincheng

Program: USG/Postbac

School: University of California, San Diego

PAD/Group: PADSTE/MPA-11

Mentor: Pantea, Cristian, MPA-11

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26678

Automated Ultrasound Data Acquisition and Analysis

The field experiments conducted by MPA-11's Acoustics Lab often require rugged, portable devices for making measurements. Additionally, memory-efficient saving capabilities are highly desirable in a field environment. An automated ultrasound data acquisition and analysis application for determining the speed of sound of a medium has been created in LabView for TiePie's Handyscope HS5, a small palm-sized device that serves as both an arbitrary waveform generator and an oscilloscope. The application is capable of generating arbitrary waveforms with nine different shapes through user defined parameters. Based on the source waveform and a basic knowledge of the system to be measured (e.g. dimensions, material properties), the application analyzes data in real-time, displaying data in both the time and frequency domains. Two different methods for sound speed calculation are employed with automatic corrections implemented for reservoir wall transit time, (1) cross-correlation and (2) de-chirp. To test the accuracy of the device and application, a measurement of the speed of sound of water at room temperature contained in a stainless steel reservoir was made using two different waveforms. The first was a wavelet with a Gaussian shaped frequency content and the second signal was a "chirp," with the frequency increasing over the duration of the signal. Results from both waveforms as well as the two data analysis methods are presented. The determined sound speeds were all found to be within 1% of accepted literature values.

Student(s): Kelso, Kwyntero Van

Program: USG/Postbac

School: Alabama A&M University

PAD/Group: PADSTE/P-24

Mentor: Venhaus, Tom, MST-16

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-25472

Analysis of Hydrogen by Time-of-Flight SIMS

Time-of-flight secondary ion mass spectroscopy (ToF-SIMS) is one of the few surface science techniques capable of detecting hydrogen. Plutonium (Pu) metal is known to contain small amounts of hydrogen in the metal matrix and likely within the oxide layer, and it is of interest to map the location of that hydrogen with ToF-SIMS as it may affect the overall corrosion behavior of the metal. To aid in the study of hydrogen in Pu, this project will create a hydrogen standard to better understand the sensitivity and uncertainty of hydrogen measurements with ToF-SIMS. A polycrystalline foil of tantalum with a thin oxide (Ta₂O₅) will be used as a target for hydrogen ion implantation. Stopping and Range of Ions in Matter (SRIM) will be used to determine energies for a desired implantation depth. Hydrogen ions will be implanted using a 200 kV DF-3000 Varian production ion implanter at the Ion Beam Materials Laboratory at LANL. The implantation profile will be verified with nuclear reaction analysis (NRA) using the ¹H (¹⁵N, α) ¹²C reaction. The results from series of ToF-SIMS depth profiles will be compared with the simulations and the NRA data. Additionally, the hydrogen detection limits for ToF-SIMS will be explored through the analysis of erbium and erbium dideuteride (ErD₂) thin films.

Student(s): Lai, You

Program: GRA

School: Florida State University

PAD/Group: PADSTE/MPA-MAG

Mentor:

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-25490

Tuning the ferromagnetic tri-critical point and quantum critical point in Ce(Pd_{1-x}Ni_x)₂P₂ under high magnetic fields

Single crystals of the substitution series Ce(Pd_{1-x}Ni_x)₂P₂ uncovered a ferromagnetic quantum critical point in the T-x phase diagram, showing a breakdown of Fermi liquid behavior, signaling the influence of quantum fluctuations. BKT theory predicts that for clean systems there is a tri-critical point that separates a high temperature line of second order phase transitions from a low temperature line of first order phase transitions, where the application of a magnetic field produces wing-like second order phase boundaries that intercept zero temperature. With increasing disorder, the tri-critical point is pushed towards zero temperature, and eventually the second order phase boundary extends all the way to zero temperature. This has spurred interest in ferromagnetic quantum criticality in disordered metals, where an intriguing possibility is that they might host anomalous metallic states and even unconventional superconductivity. Ce(Pd_{1-x}Ni_x)₂P₂ provide a new platform for addressing this picture, where it is possible to systematically vary the Curie temperature and the chemical disorder and track the evolution of the tri-critical point, and the quantum critical region. We will measure magnetoresistance, torque magnetometry, and extraction magnetometry for Ce(Pd_{1-x}Ni_x)₂P₂ using pulsed field facility at LANL.

Student(s): Murphy, Eamonn Conor

Program: Post Masters

School: Imperial College London

PAD/Group: PADSTE/C-CDE

Mentor: Labouriau, Andrea, C-CDE

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26385

Improving the Properties of Sylgard 184

Improving the Properties of Sylgard 184 Sylgard 184 is a commercial PDMS-based polymer that is extensively used for microfluidics, micro-engineering applications, the protection of electrical devices and more generally as a potting material. [1] The removal of cured Sylgard 184 and other PDMS based resins is arduous without the use of mechanical scraping, water rinsing, or the use of organic solvents, which is not suitable for all applications. [2] Additionally, the curing time for Sylgard 184 is relatively slow and requires approximately 24 hours at room temperature. [3] In temperature sensitive applications, it is desirable to accelerate the curing time while remaining at room temperature. In this work, we will investigate the reduction of the curing time at room temperature, while studying the impact of various fillers on the bonding properties on different surfaces. Moreover, because of its use as a potting material, it is crucial to evaluate its water absorbing-repelling characteristics and how the addition of fillers allows for protection of the water sensitive surface. The chemical, thermal and mechanical properties of the modified Sylgard 184 will be studied using Fourier-transform infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), microscopy, tension and hardness tests.

Student(s): Rietema, Connor James

Program: GRA

School: Colorado School of Mines

PAD/Group: PADSTE/MST-8

Mentor: Saleh, Tarik A, MST-8

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-25617

Microstructure and Texture Analysis of Cold Formed Nanostructured Ferritic Alloys

Generation IV nuclear reactors demand materials able to withstand extreme irradiation over a wide range of temperatures. Alloy 14YWT is under development for use as cladding in Gen IV sodium fast reactors. The alloy is a nanostructured ferritic alloy (NFA) characterized by a dense dispersion of nano-oxides (NOs) usually in the form of Y-Ti-O clusters ranging in size from 1-10 nm in diameter. The NOs give the alloy a high degree of irradiation resistance and thermal stability. Two heats of 14YWT studied, CEA 14YWT and FCRD NFA-1. Both alloys were gas atomized, mechanically alloyed as powders, then consolidated using either hot extrusion (FCRD NFA-1) or hot isostatic pressing (CEA 14YWT). Seamless tubes were machined from the consolidated material to be cold reduced to final dimensions. Two cold forming methods were attempted, hydrostatic extrusion (HE) and pilger processing. Both the CEA 14YWT and FCRD NFA-1 were formed with HE while only the FCRD NFA-1 was pilgered. Microhardness was measured post processing and also after the first pilger pass. Electron backscatter diffraction (EBSD), orientation imaging microscopy (OIM), and pole figures were used to investigate the microstructures and determine the cause of the large spread in hardness observed for FCRD NFA-1 and the drop in hardness of the pilgered material. The low final hardness of the pilgered material was due to in part to excessive grain growth during the high temperature anneal. The repeated heat treatments at 1200°C between passes may have coarsened the NOs, resulting in the rapid grain growth. The spread in hardness of FCRD NFA-1 caused by the bimodal grain size of the starting material is not reduced by either forming process. The texture of the pilgered material varied substantially from the HE material. This could impact the anisotropy of the mechanical properties.

Student(s): Rubio, Natalia Leonie

Program: USG/Postbac

School: University of California Berkeley

PAD/Group: PADSTE/MST-8

Mentor: Maloy, Stu, MST-8

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26131

Studies of Corrosion Resistant Materials Exposed to High Temperature Lead-Bismuth Eutectic

This work investigates several corrosion-resistant materials for their compatibility with high temperature lead-bismuth eutectic. Materials studied included various refractory metals and steels. Samples were submerged in molten lead-bismuth and the resulting corrosion damage was analyzed via SEM and EDS. When applicable, the interfaces were inspected for the formation of protective oxide layers.

Student(s): Sakano, Michael N

Program: GRA

School: Purdue University

PAD/Group: PADSTE/T-1

Mentor: Kober, Ed, T-1

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26288

Comparison of Reduced Chemistry models for RDX and HMX

“Reduced order” chemistry models using the non-negative matrix factorization algorithm are developed for RDX, and differences compared to HMX are presented under various small-scale temperature and pressure homogeneous isothermal simulations. The initial decomposition of RDX using the ReaxFF-Ig force field parameterization begins with primarily NO₂ dissociation and concurrent HONO elimination. HMX, being a strained eight-membered nitramine, also decomposes from some ring-break mechanisms, in addition to the two previously mentioned pathways. Generalization of these chemical vectors are then applied to larger multi-million atom simulations represented by 1-D Cook-off growth, shocked gaps and, thermostatted hot spots. Variations in chemistry are noted and might provide further understanding for the differences between RDX versus HMX, homogeneous heating versus 1-D gaps, and hot spots forming from thermostating versus shock-induced collapse. Finally, there will be a brief discussion considering implications of applying classical thermal conductivity, as well as providing comparisons with already established reaction mechanisms from both simulations and experiments.

Student(s): Stupka, Richard Dylan

Program: USG/Postbac

School: New Mexico State University

PAD/Group: PADSTE/SIGMA-2

Mentor: Nolen, Blake Penfield, SIGMA-2

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26458

Evolved Hydrogen gas analysis using RGA

Fine metal powders, such as Tantalum and Aluminum can oxidation and evolve Hydrogen gas when exposed to water. When these materials are confined to a sealed container such as a waste barrel, evolved hydrogen gas among other gaseous effluents can pose a pressure and fire issue. Mineral oil compounds like Hysol™ are added to such mixtures to mitigate oxidation and reduce production of hydrogen gas. An experiment was designed to mix micron length metal filament powders with water and Hysol™ to see the rate at which hydrogen gas and other gaseous effluents evolve with the addition of Hysol™ to the mixture. After establishing a baseline measurement with just water and Hysol™, different metal powders were added to the mixture to see which evolved hydrogen and at what rate. The metals used were; Aluminum, Tantalum, Stainless Steel and Titanium. The ratio of water to Hysol™ was kept constant once a baseline was established. The volume of evolved Hydrogen gas was measured using a Residual Gas Analyzer (RGA). The RGA plotted the atomic mass of the gaseous compounds in the sample (x-axis) with respect to the partial pressures of those compounds (y-axis) over time. The goal of this experiment was to determine the ideal concentrations of metal powder waste, which can be safely stored in the water/ Hysol™ mixture, thus preventing a hydrogen overpressure issue in waste drums.

Student(s): Turman, Haley Brooke

Program: GRA

School: Texas A&M University

PAD/Group: PADSTE/AOT-MDE

Mentor: Woloshun, Keith Albert, AOT-MDE

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26364

Investigation of the Effect of Annealing on Irradiated Alloy 718

During normal accelerator operations at the Isotope Production Facility (IPF) within the Los Alamos Neutron Science Center (LANSCE), an Alloy 718 beam window can have fluctuations in temperature of up to 100C. The effects of these fluctuations can anneal radiation damage and possibly cause precipitation of other phases. This study aims to systematically determine the effects of deliberate temperature excursions on the microstructure of irradiated Alloy 718 starting in the annealed condition. This will be accomplished by characterizing the properties of a set of Alloy 718 samples at three annealing conditions (room temperature, 100 C, and 200 C), and two irradiation doses (1 dpa and 15 dpa). Each condition will be compared with virgin annealed Alloy 718. Microstructural evolution, including precipitate size, density, and crystallinity, will be analyzed with a Transmission Electron Microscope (TEM). Additionally, nanohardness and nanopillar testing will be carried out on the relevant samples.

Student(s): Wilson, Tashiema Lixona

Program: GRA

School: University of South Carolina

PAD/Group: PADSTE/MST-8

Mentor: White, Joshua Taylor, MST-8

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-25957

Understanding Uranium Silicide Fuel and the effects of Fission Products

The push to develop new fuel types for use in current light water reactors (LWR) is driven by the need for accident tolerant fuels (ATF) that exhibit improvements in operational and transient safety. Among the candidates are uranium-silicide compounds, most notably U_3Si_2 due to its increased U-density and higher thermal conductivity. While the system has been well-studied, uncertainties remain concerning structures and stoichiometries of solid solution phases. Furthermore, the effect of burnup has not been thoroughly investigated. During burnup many different types of fission products are formed which will affect the morphology of the fuel, hence affecting the thermophysical properties. In this study, compositions between U_3Si_2 and USi_3 were fabricated by arc-melting. In addition, the impact of the dominant fission products that form during the life-cycle of a fuel element were systematically studied by arc-melting. Analyses included x-ray diffraction, high temperature neutron scattering, scanning electron microscopy with energy dispersive spectrometry and polarizing light microscopy, and identification of phase transitions using differential scanning calorimetry. The results from this study allows for a new interpretation of the U-Si phase diagram.

Student(s): Yang, Michelle H

Program: USG/Postbac

School: UC Berkeley

PAD/Group: PADSTE/MST-7

Mentor: Yang, Dali, MST-7

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26327

Comparing Different Techniques to Analyze the Thermal Degradation of Nitroplasticizer Aged with Vinyl Copolymer Elastomer

Nitroplasticizer (NP), a eutectic mixture of bis(2,2-dinitropropyl) acetal (BDNPA) and formal (BDNPF), is an essential component to a binder used in PBX formulations. Previous studies show NP's decomposition at elevated temperatures creates reactive byproducts that can compromise mechanical and chemical properties of other components in PBX, but few explore how degradation of other components impacts characteristics of NP. In this study, NP samples were exposed to either 100% vinyl copolymer elastomer (VCE) or 50%VCE/50% filler at 3 different temperatures (38C, 55C, 70C) for 2 years. Changes in composition of the NP samples were analyzed using different instrumentations, such as refractometry, UV-Vis, TGA, and FTIR. When aged at low temperatures, little change occurred in the UV spectrum or refractive index of aged samples compared to that of a baseline NP. However, when the samples were aged at 70°C, differences in refractive index, TGA, UV-Vis, and FTIR results are drastic. Further comparison with NP aged under N₂ at the same temperatures using FTIR indicates the presence of VCE plays a key role in determining the rate and mechanisms of NP during the thermal aging process. These different techniques provide unique insights on NP thermal aging.

Student(s): Zhao, Jianchao

Program: USG/Postbac

School: University of Louisville

PAD/Group: PADSTE/C-CDE

Mentor: Lee, kwan, C-CDE

Category: Materials Science

Type: Individual Poster

LA-UR: LA-UR-18-26401

Effect of Surface Area of Silica Fillers in PDMS-based 3D Printable Ink Formulation

Additive manufacturing (AM) is an emerging research field due to its ability to manufacture materials with controlled geometry and properties using computer-based 3D printing technology. Currently, the main challenge with this technology deals with limited materials, or ink, available for processing, specifically in the field of polymers. PDMS (silicone) is one of the most commonly used elastomers in a variety of applications, including microfluidic fabrication, medical devices, and soft electronics. Due to its low-cost, backbone flexibility, low intermolecular interactions and chemical inertness, PDMS has become an attractive material for AM and 3D printing applications. Here, we have developed PDMS-based 3D printable resin formulations with silica fillers that exhibit different surface areas. Additionally, we studied the surface area effect of the silica fillers on the ink formulations as well as on 3D printed product, using rheological analysis as well as thermal and mechanical characterization.

Mathematics

Student(s): Martinez, Kaitlyn

Program: GRA

School: Colorado School of Mines

PAD/Group: PADSTE/T-6

Mentor: Manore, Carrie Anna, T-6

Category: Mathematics

Type: Individual Poster

LA-UR: LA-UR-18-26072

Evaluating Risk of Mosquito Borne Viruses in Brazil

Mosquito-borne diseases such as newly emergent Zika (ZIKV) and Chikungunya (CHIKV) and endemic Dengue (DENV), have presented significant challenges to the public health community in Brazil, and we do not yet fully understand the dynamics of these diseases. Due to this shortcoming, it is challenging to combat, control or prevent the spread of ZIKV, CHIKV, and DENV in the region. All three viruses are spread primarily by the *Aedes aegypti* mosquito. CHIKV and ZIKV can be asymptomatic and are often misdiagnosed, and each virus has heterogeneous incidence rates over the entire country, so it is not clear what factors in the human population and the environment contribute significantly to the proliferation of each virus. Consequently future intervention strategies and prevention techniques may not be targeted at the most effective areas of risk mitigation. In this project we will determine the demographic and environmental factors that correspond to the highest level of risk for each disease using Multivariate Regression and Clustering Analysis at four different spatial discretization levels. We have discovered that one single factor does not drive viral incidence; instead, there are groups of factors that in conjunction predict viral incidence. By comparing these groups of predictors across disease type, we can show which predictors are invariant across disease and thus correspond to universal mitigation strategies as well as those factors unique to the disease and thus necessitate targeted intervention.

Student(s): Rajadhyaksha, Aditi Milind

Program: USG/Postbac

School: University of Michigan

PAD/Group: PADSTE/CCS-6

Mentor: Casleton, Emily Michele, CCS-6

Category: Mathematics

Type: Individual Poster

LA-UR: LA-UR-18-25412

Assessing Reactor Operation through Imagery of the Cooling Tower Plume

Multi-Informatics for Nuclear Operations Scenarios (MINOS) is a multi-laboratory venture that aims to combine different data streams to form a unified conclusion about the state of operations at a facility. The overall mission is to use data fusion to support nuclear proliferation detection. To achieve this goal, MINOS monitors the High Flux Isotope Reactor (HFIR) and Radiochemical Engineering Development Center (REDC), a research reactor and reprocessing facility at Oak Ridge National Laboratory. HFIR is a high flux reactor-based neutron source. It operates at 85 megawatts, produces various isotopes, and is used for research in several different fields. The REDC is a radiochemical processing and research facility that produces radionuclides that are used for various applications. MINOS uses several different data modalities to answer fundamental questions about the state of operations at the HFIR-REDC facility. The data modality I explored during my internship is imagery of HFIR's cooling tower plume. The objective is to use these images to identify characteristics that could indicate the state of HFIR independent of any other information. Some questions that these images can potentially address include: Can the power production of HFIR be estimated? What is the schedule of operations? Is an unknown activity power-intensive? What is the production rate? Once a method is found to answer these questions using the cooling tower plume imagery, ground truth data will be used to confirm predictions from the plume imagery. The goal is for this method to be used in conjunction with the other data modalities. The combination of information from the different data sets will be used to characterize operations at HFIR-REDC. This system may be applied to other facilities to reduce uncertainty in nuclear proliferation detection operations.

Other

Student(s): Roy, Avipsa

Program: GRA

School: Arizona State University

PAD/Group: PADSTE/CCS-6

Mentor:

Category: Other

Type: Individual Poster

LA-UR: LA-UR-18-25465

Geographic visualization to identify features from LiDAR point clouds

The recent advances in geographic data collection have rapidly changed visualizing spatial information. Integrating light detecting and ranging (LiDAR) into mobile mapping systems have allowed for a new horizon in determining signatures from geotagged images. The LiDAR point clouds combined with simple meshes can help to discover features that inform the state of facility operations in and around building structures by examining elevation, temperature and intensities associated with each block of the facility. Our study area is the open research nuclear reactor called High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory in Oak Ridge, Tennessee. The broader goal of the research encompasses an NA-22 effort called MINOS (Multi Informatics for Nuclear Operation Scenarios), meant to use data analytic tools to characterize activities within a nuclear facility by studying a variety of sensors placed around it. Our objective is to perform an exploratory analysis to understand and identify informative signatures in and around the HFIR Facility from the multiple spatial modalities (point clouds, thermal imagery) captured by the VLP-16 LiDAR unit. We use ECHO as a tool to store and analyse our data. Imagery analysis and anomaly detection is carried out using QGIS and Python.

Physics

Student(s): Bao, Brandon Jemez

Program: USG/Postbac

School: University of California, San Diego

PAD/Group: PADSTE/AOT-RFE

Mentor: Scheinker, Alexander, AOT-RFE

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26435

Convolutional Neural Networks for Finding Control Parameters

Particle accelerators create intense, high energy beams which can be directly used for research, such as proton radiography at LANSCE, or which can generate short, bright flashes of light, such as at Stanford's Free Electron Laser, LCLS. Intense charged particle beams undergo complex nonlinear dynamics and are accelerated via thousands of coupled electromagnetic components which make up the accelerators, all of which drift unpredictably with time. It is challenging to precisely control and quickly tune the phase space distributions (energy spread, current profile, etc.) of such beams. The goal of this work is to study the possibility of applying convolutional neural networks for mapping 2D phase space measurement images of electron bunches to particle accelerator component settings. This is one of the initial steps towards achieving automatic control and tuning of such beams. Convolutional Neural Networks (CNN) are an effective tool for image processing, allowing for multi-parameter regression. Images are first preprocessed and normalized before being input into the network. In convolution layers, filters slide over images to identify important features. Nonlinearity is introduced via various layers including rectified linear units (ReLU) or sigmoid functions. Pooling layers reduce dimensionality of the network, keeping only the important features. This cycle of layers repeats in the network for the desired complexity of a problem until the final layer outputs predicted values for regression. Before moving to real data, a simple network was first created to find the radii of images of circles of varying intensity, proportional to their areas. The complexity of the problem was incrementally increased by finding major and minor axes of ellipses, adding noise, and random rotations before moving on to collected electron beam data. The goal was for the network to predict parameters with an error variance of 1% and mean of 0.1%.

Student(s): Cassidy, Mary Clare

Program: USG/Postbac

School: United States Military Academy - West Point

PAD/Group: PADSTE/P-21

Mentor: Boshier, Malcolm Geoffrey, P-21

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26013

It's Time to Split: Modeling the Splitting of Ultra Cold Atoms Using Standing Light Waves

Ultra cold atoms can improve accelerometers and gyroscopes, ultimately producing more precise sensors. These sensors are based on atom interferometry, which splits and recombines ultra-cold atoms, then compares the differences between the original and final states. When atoms are cooled to almost absolute zero, their wave-like property becomes more prominent, resulting in matter waves. In interferometry, matter waves generate greater sensitivity than electromagnetic waves, and thus are optimal for use in sensing. However, splitting matter waves is different than splitting laser beams. One way to split ultra-cold atoms is a standing light wave. Using Schrodinger's Equation, I am simulating the separation of one group of ultra-cold atoms, also referred to as a Bose-Einstein Condensate (BEC). When the BEC separates, it is sent into different momentum states moving in opposite directions. Using a mirror wave pulse similar to the separation pulse, I model the reversal of the states' momenta, causing the wave packets to move towards one other. Finally, a recombination wave pulse can be used to bring the BEC back to the original state. In totality, this process will simulate an atom interferometer. I hope to explore different momentum states and varying initial BEC velocities to eventually explain behavior seen in actual experiments. In this poster I will present my work thus far.

Student(s): Danielson, Daine Lee

Program: USG/Postbac

School: University of California, Davis

PAD/Group: PADSTE/T-2

Mentor: Hayes-Sterbenz, Anna Catherine, T-2

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-23776

Reactor Neutrino Spectral Distortions Play Little Role in Mass Hierarchy Experiments

The Coulomb enhancement of low energy electrons in nuclear beta decay generates sharp cutoffs in the accompanying antineutrino spectrum at the beta decay endpoint energies. It has been conjectured that these features will interfere with measuring the effect of a neutrino mass hierarchy on an oscillated nuclear reactor antineutrino spectrum. These sawtooth-like features will appear in detailed reactor antineutrino spectra, with characteristic energy scales similar to the oscillation period critical to neutrino mass hierarchy determination near a 53 km baseline. However, these sawtooth-like distortions are found to contribute at a magnitude of only a few percent relative to the mass hierarchy-dependent oscillation pattern, both in energy space and in Fourier space. In the Fourier cosine and sine transforms, the features that encode a neutrino mass hierarchy dominate by over sixteen (twenty-five) times in prominence to the maximal contribution of the sawtooth-like distortions from the detailed energy spectrum, given $\Delta E_{\text{res}} = \sqrt{E_{\text{vis}}} = \text{MeV}$ (perfect) detector energy resolution. The effect of these distortions is shown to be negligible even when the uncertainties on the reactor spectrum, oscillation parameters, and counting statistics are considered. This result is also shown to hold even when the opposite hierarchy oscillation patterns are nearly degenerate in energy space, if energy response nonlinearities are controlled to below 0.5%. Therefore with accurate knowledge of detector energy response, the sawtooth-like features in reactor antineutrino spectra will not significantly impede neutrino mass hierarchy measurements using reactor antineutrinos.

Student(s): Davie, Kayla Diann

Program: GRA

School: University of Maryland-College Park

PAD/Group: PADSTE/T-1

Mentor: Zammit, Mark Christian, T-1

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26278

Low-Density Plasma Modeling Utilizing Maxwellian and Non-Maxwellian Electron Energy Distributions

Plasma modeling requires the calculation of rate coefficients for the determination of atomic and molecular populations, which allows the calculation of plasma properties such as radiative power losses, opacity, etc. In order to model low-density plasmas, we calculate rate coefficients assuming Maxwellian and non-Maxwellian distributions of electron energy. For this project, we have written a code to calculate rate coefficients using both Maxwellian and non-Maxwellian distributions for modeling low-density plasmas such as primordial gas clouds in the interstellar medium and magnetically confined fusion plasmas. During this presentation, I will talk about the concepts of modeling low-density plasmas utilizing ab initio approaches, and investigate the validity of the semi-empirical formula utilized in LANL Atomic Physics Codes for representing the energy-sharing distribution associated with the process of electron-impact ionization.

Student(s): Erickson, Onnolee Ima Englert

Program: USG/Postbac

School: Stony Brook University

PAD/Group: PADSTE/P-23

Mentor: Gehring, Mandie, P-23

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-25826

Creation of a Database to Determine the Effective Cross Sections of Materials

This project created a way for the neutron-interaction cross sections of a compound to be found quickly and easily using isotope cross section data and Matlab. To determine the elemental cross sections, every isotope cross section that shares the same element was multiplied by its natural isotopic abundance and added together. Then each element of the compound of interest is multiplied according to its stoichiometric ratio, and finally constituent element contributions are summed. The cross section data (barns), collected from the Evaluated Nuclear Data File (ENDF), and its corresponding incident energy level were interpolated using Matlab to create a standard range of energy values that was used for every isotope included in the database. For the first fifty elements and their isotopes, I used this method to determine the cross section of each isotope in the energy range of 10^{-5} eV to 20 MeV. Then, the interpolated cross sections were multiplied by their natural abundance. This created the data used to derive the effective cross section of an element. The process is repeated using the element cross sections and their ratios within the substance to determine the cross section of the compound. I will present details of the calculation and an example of the database's usefulness - a comparison of the (n,gamma) cross sections for a variety of detector compounds of interest to my team.

Student(s): Haffey, Kiersten Elizabeth

Program: GRA

School: University of California-San Diego

PAD/Group: PADSTE/P-21

Mentor: Nath, Pulak, P-21

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-21228

Towards the Development of a Platform for Single Cell Analysis

Single cell analysis of genomics, transcriptomics, proteomics and metabolomics requires a method to isolate, manipulate, and visualize nano-liter samples. Current microfluidic methods to capture single cells such as in hydrodynamic traps, or dielectrophoretic traps do not typically facilitate serial processing such as transfection, lysis, washing, and DNA/protein extraction. Additionally, these methods have limited capabilities to deterministically release the processed sample for further off-chip processing. In this work, we present a novel microfluidic platform that can facilitate in situ processing and analysis of a nanoliter sample by trapping, delivering serial reagents, and rapidly mixing in a seamless, continuous operation. This platform is composed of microfluidic traps placed along a microchannel. The traps are comprised a thin semipermeable membrane separating a pneumatic control channel and a fluid channel. Actuation of the membrane can draw sample from and return the sample to the microchannel. The semipermeable membrane allows air within the fluid channel to escape. Plugs of aqueous solutions are created in the central channel such that nano-liter samples can be withdrawn into the traps by the actuation of the membrane. Plugs with different solutions are created in a series such that mixing can take place between the sample and aqueous plugs as the plugs move passed a trap. This enables automation of serial operations on the nano-liter sample. By altering parameters such as size of traps, plug size and flow rates, the mixing speed and sample preservation can be optimized for a specific application. The device is fabricated using a laser based micro-patterning and lamination method which facilitates the ability to install difficult-to-handle, thin, stretchable, semipermeable membranes. Initial proof of principle is demonstrated using food coloring dye and particles. With further customization of the nano-liter microfluidic platform, we envision diverse applications for single-cell isolation, manipulation and analysis in a single, simple platform.

Student(s): Hayes, Brandon Shafer

Program: USG/Postbac

School: Rochester Institute of Technology

PAD/Group: PADSTE/P-21

Mentor: Nath, Pulak, P-21

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26240

Particle/Cell Ordering Using Inertial Focusing in Spiral Microchannels

Single cell analysis involves capturing individual cells for a wide range of biological applications. We have developed a unique microfluidic single cell trap array integrating elastic membranes that can be actuated for active cell trapping and manipulation. Currently, a single cell trapping efficiency of less than 20% has been achieved by utilizing extremely dilute samples. This work applies particle ordering via inertial focusing to increase the single cell trapping. Inertial focusing relies upon hydrodynamic effects in order to focus and order particles in spiral microfluidic channels. Although still in the laminar regime, Reynolds number in the range of 1-100 requires the consideration of inertial effects – unlike conventional Stokes flow in microfluidics. Using a rapid prototyping method based on laser micro-patterning and lamination, a spiral microfluidic device was fabricated with 100 μm x 40 μm channel cross-sectional area to analyze the extent of particle ordering. High speed imaging was utilized to visualize particle ordering (4000 fps); to quantify the ordering, custom MATLAB scripts were developed to perform particle tracking based on a MATLAB implementation of the IDL (Interactive Data Language) particle tracking algorithm. After image processing, more than 30,000 frames were analyzed to determine particle ordering statistics and an average particle spacing distance. Using this approach the distance between traps can then be designed such that each trap isolates a single particle/cell from the ordered particle train to considerably enhance single cell trapping efficiency.

Student(s): Hurd, Sara Jean

Program: USG/Postbac

School: New Mexico State University

PAD/Group: PADSTE/P-21

Mentor: Boshier, Malcolm Geoffrey, P-21

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26280

Optimum Transportation of Cold Atoms

When atoms become extremely cold, they form a new state of matter known as a “Bose-Einstein condensate” (BEC). Atoms in this state are useful for making sensors because microscopic quantum phenomena, particularly wave function interference, become apparent. This can be exploited to build ultra-sensitive navigation systems that avoid reliance on the commonly used Global Positioning System (GPS). The cooling method that brings the atoms’ state to BEC is multistage process, in which lasers are used to slow the atoms down. A laser photon colliding with an atom moving in the opposite direction will cause it to slow down. Once the atoms are cooled in this way, they have to be moved to a different part of a vacuum system. This is done by trapping them in a focused laser beam using their electrical polarizability and moving the focal point. My project is to optimize this transport process to minimize energy gain and atom loss. I am simulating this process using classical mechanics to describe the dynamics of the atoms in the moving laser trap. In this poster, I will present my progress towards the goal of optimum transport.

Student(s): Lambert, Jared Campbell

Program: USG/Postbac

School: Utah State University

PAD/Group: PADSTE/P-25

Mentor: Tang, Zhaowen, P-25

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-25540

Ultra-Cold Neutron measurement of Proton branching in neutron Beta decay (UCNProBe)

The lifetime of the free neutron has been measured many times, each experiment using one of two methods: measuring the decay products of neutrons in a well calibrated neutron beam (beam experiment), or counting the number of surviving neutrons stored in a UCN trap over time (bottle experiment). The lifetime results from the two different methods of experiments differ by 10 seconds or five standard deviations. Our goal is to resolve the difference between the two measurements by measuring the proton branching ratio of neutron decay using UCNs. Detecting a proton branching ratio of less than one will indicate new physics beyond the Standard Model of particle physics. The experiment is realized by storing the neutrons in a scintillating material trap. To measure the proton branching ratio, we will attempt to measure the absolute number of UCNs inside the trap and the absolute number of electrons from beta decay to 0.1% precision. Through simulation we have determined that a measurement of 0.1% will be possible.

Student(s): LaRose, Ryan

Program: GRA

School: Michigan State University

PAD/Group: PADSTE/NSEC

Mentor: Coles, Patrick Joseph, T-4

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-25861

Quantum Assisted Quantum Compiling

Compiling quantum algorithms for near-term quantum computers (accounting for connectivity and native gate alphabets) is a major challenge that has received significant attention both by industry and academia. Avoiding the exponential overhead of classical simulation of quantum dynamics will allow compilation of larger algorithms, and a strategy for this is to evaluate an algorithm's cost on a quantum computer. To this end, we propose quantum-assisted quantum compiling (QAQC). In QAQC, we use the Hilbert-Schmidt inner product between a target unitary and a trainable unitary as the cost function to be evaluated on the quantum computer. We introduce two circuits for evaluating this cost. One circuit computes the magnitude of the Hilbert-Schmidt inner product and we use this circuit for gradient-free compiling. Our other circuit gives the real and imaginary parts of the Hilbert-Schmidt inner product and is a generalization of the Power of One Qubit that we call the Power of Two Qubits. We use this circuit for gradient-based compiling. As a demonstration of QAQC, we compile various one-qubit gates on IBM's and Rigetti's quantum computers into their respective native gate alphabets. Future applications of QAQC include algorithm depth compression, black-box compiling, noise mitigation, and benchmarking.

Student(s): Maez, Colin Joshua

Program: High School

School: Santa Fe Community College

PAD/Group: PADSTE/P-23

Mentor: Duke, Dana Lynn, P-23

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-25963

Collimation Design for a Deuterium-Tritium Neutron Generator

With the commission of the Thermo Fisher's Scientific MP 320 DT Neutron Generator at TA-53, design and construction of collimation shielding is required. The Deuterium-Tritium (DT) Neutron Generator produces gamma and neutron radiation (13-15 MeV) into a 4π solid angle, thus the collimation needs to forward-direct neutrons for experimental efforts. The main purpose of the shielding is to channel and dissipate the anisotropic neutrons produced by the generator. An analysis of the shielding material properties, measurements of the time of flight (TOF), neutron flux, room geometry and an understanding of the generator were all needed to draft a schematic. Once the schematic was approved, construction began. This analysis and implementation will be presented. The future application of the DT Neutron Generator is to provide a detector development test station for Neutron Diagnosed Subcritical experiments (NDSE), a 3D neutron imaging capability at the National Ignition Facility (NIF), and diagnostics development for nuclear data.

Student(s): Mendoza, Emily Faith

Program: High School

School: New Mexico Highlands University

PAD/Group: PADSTE/P-23

Mentor: Briggs, Matt, P-23

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-25949

Simulation Of Neutron Scattering In Inertial Confinement Fusion Implosions To Improve 3D Cold Fuel Reconstruction

At the National Ignition Facility (NIF) a plastic capsule filled with Deuterium and Tritium (DT) fuel is compressed using indirect laser drive to achieve nuclear fusion. The neutron imaging team takes pictures of this Inertial Confinement Fusion (ICF) implosion using the neutrons emitted in the fusion reactions. The images are taken with a gated system to allow neutron energy selection based on time-of-flight. The primary picture records both the size and shape of the burning fusion fuel (14.1 MeV) at stagnation, while the second image taken shows the low energy neutrons (6-12 MeV) that scatter in the surrounding cold fuel. We create a radiation transport simulation of the burning fuel assembly to study angular and energy distributions of neutrons scattering in the cold fuel. The simulation results will aid in creating an accurate three-dimensional reconstruction of the complete fuel assembly including cold fuel density.

Student(s): Peets, Emrys b

Program: USG/Postbac

School: University of Texas at Austin

PAD/Group: PADSTE/P-23

Mentor:

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26055

Neutron Yield and Energy Characterization for a Dense Plasma Focus DD Source

Dense Plasma Focus (DPF) devices generate various forms of electromagnetic radiation and fusion byproducts through the rapid ionization (and ablation) of the deuterium based gas located in the device. Study of the yield of these devices has important scientific and industrial rooted consequences. A DPF Deuterium-Deuterium sourced device, located in Albuquerque, New Mexico, has an estimated neutron yield of 10^{14} 2.45 MeV neutrons per pulse. The experimental set up includes a silver activation foil, and a Geiger-Mueller based detection system. Geiger-Mueller systems, unfortunately, do not provide insights into the energy spectrum of the generated neutrons nor are they typically used in instances of such high yield. As such, it is necessary to characterize the DPF source through alternative means. The purpose of this study is to determine the neutron yield of this device using different activation techniques, and also provide a characterization of the temporal pulse of the neutrons emitted with a scintillator based detection system. With this alternative method of detection, we are able to provide further insights into the capabilities of DPF devices. In the near future, these measurements will be compared with a higher yield deuterium-tritium source.

Student(s): Robles, River Robert

Program: USG/Postbac

School: University of California, Los Angeles

PAD/Group: PADSTE/AOT-AE

Mentor: Anisimov, Petr Mikhailovich, AOT-AE

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26215

Increasing High-Energy XFEL Efficiency with a Transverse Gradient Undulator

In this poster we explore challenges associated with the design of high-energy x-ray sources and present one possible design method for a future source here at LANL, MaRIE (Matter-Radiation Interactions in Extremes). The success of the project would allow breakthroughs in dynamical imaging of high-Z materials under extreme conditions. Current x-ray sources are incapable of probing these environments, restricting the potential for scientific discovery. MaRIE's higher photon energies would reach this regime and would be, to date, the only 42+keV light source to produce enough photons for dynamical imaging. It employs the free electron laser (FEL) process, in which an electron beam is inserted into a magnet array after compression in a beamline, with the subsequent motion causing the beam to radiate coherently. FEL efficiency breaks down at high energies because of energy spread increases that occur during compression, requiring a new beam delivery scheme for 42+keV sources. We alter a mechanism known as phase-merging enhanced harmonic generation (PEHG), which compresses within the periods of a seed laser, avoiding ordinary degradation problems by reducing the strength of the compressing elements for the purpose of the beam delivery. The success of this scheme would allow MaRIE to deliver the promised photon quantity and reveal a new frontier to the scientific community.

Student(s): Sorenson, Josef Daniel

Program: USG/Postbac

School: University of New Mexico

PAD/Group: PADSTE/P-25

Mentor: Durham, Matt, P-25

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26429

Using Muon Tomography to Identify Features of Interest in Reinforced Concrete Structures

In New Mexico and around the country there is an abundant problem where engineers do not know the structural details of old bridges. Most methods to image the bridges either cannot penetrate the thick concrete (i.e. X-Ray) or have other problems. We constructed a segment of a supporting column based on a Pennsylvania DOT reinforced concrete pier standard and used muon tomography to image the model. Our simulation and preliminary results show that muon tomography is an excellent candidate for identifying points of interest in reinforced concrete.

Student(s): Stiftel, Justine Gabrielle

Program: USG/Postbac

School: Bryn Mawr College

PAD/Group: PADSTE/AOT-AE

Mentor: Nichols, Kimberley, AOT-AE

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26190

Making mini-accelerators possible via beam shaping

Recent developments in advanced accelerators such as dielectric laser accelerators and wakefield accelerators have shown the way toward accelerators that increase affordability and access for fundamental physics research, medical procedures, and electronics production, such as millimeter scale projects like Accelerator on a Chip. Their promising future is dependent upon stability characterized by the transformer ratio (TR) of the beam. While typical beam profiles are limited to a ratio of 2 at most, with other beam shapes, such as double triangle, there is potential for higher TR. This advancement is due in part to the development of emittance exchangers (EEX), whereby the transverse particle distribution can be transformed to a longitudinal particle distribution. Design and transport of a millimeter-scale triangular shaped beam is explored through simulation of particle flight paths.

Student(s): Tafoya, Jose I

Program: High School

School: Washington University in St. Louis

PAD/Group: PADSTE/P-23

Mentor: Volegov, Petr Lvovich, P-23

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-25955

Scintillator Characterization for Neutron Imaging of Inertial Confinement Fusion Implosions

The investigation of asymmetries in inertial confinement fusion (ICF) implosions is facilitated by neutron imaging, which allows for the reconstruction of a compressed Deuterium-Tritium (DT) fuel capsule. Diagnostic analysis of hotspot and cold fuel density through gated imaging of the primary (14.1 MeV) and down-scattered (6-12 MeV) neutrons emitted by fusion reactions aids in the improvement of ICF experiments at the National Ignition Facility (NIF). Currently, two new active imaging systems are being designed for the NIF on two new lines-of-sight, in order to facilitate 3D fuel reconstruction. Neutron imaging relies on the conversion of neutrons into visible light through the use of a scintillator. To investigate the properties of new scintillator materials for possible application in ICF neutron imaging, various scintillators were tested using neutrons produced by the accelerator at the Los Alamos Neutron Science Center (LANSCE). Results of the experiments have been used to characterize scintillator spatial resolution, efficiency, and noise properties. These scintillator measurements will lead to improvements in neutron imaging system design, as well as improved data interpretation from the existing detector.

Student(s): Williams, Joseph James

Program: USG/Postbac

School: The University of Texas at Austin

PAD/Group: PADSTE/CCS-2

Mentor: Cooley, James Hamilton, CCS-2

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-25330

Atomistic Simulations and Theoretical Investigations of the Plasma Bump-on-Tail Instability

The plasma two-stream, bump-on-tail instability has been well-studied with the Vlasov-Poisson equations and other collisionless methods. This research presents the first investigation into the instability that accounts for collisional effects. This research focused on both theoretical derivations and computational results from a molecular dynamics Python code. Both the theoretical and numerical model focused on the Yukawa model of positively-charged ions shielded by an electron cloud; in both cases, an initial potential field was applied to perturb the system, and the early-time growth or decay of the stable and unstable modes of the systems were compared in dimensionless dispersion plots. Relevant parameters included the Yukawa shielding strength, the mean stream velocity, the strength of the tail, and the mode and strength of the initial perturbation. While the dispersion plots from the theoretical and computational models largely agreed, due to the discrete and finite nature of the particles in computational model, the strength of the perturbation was found to be a very important parameter in the computational model that greatly affected the growth rate of the instability.

Student(s): Zimmermann, Ingrid Hana

Program: USG/Postbac

School: Rutgers University

PAD/Group: PADSTE/MPA-MAG

Mentor: Mcdonald, Ross David, MPA-MAG

Category: Physics

Type: Individual Poster

LA-UR: LA-UR-18-26441

Developing a New Method for Torque Magnetometry

The behavior of quantum materials due to strong electronic interactions is commonly characterized by the anisotropy in spin and charge degrees of freedom. A nonzero angle between the magnetization of a crystal and an externally applied magnetic field causes a torque to be exerted on the crystal sample, which makes torque magnetometry a powerful technique for directly measuring the anisotropy of magnetization. Piezoresistive cantilevers, tools for torque magnetometry, are in limited commercial supply. We are developing a torque magnetometer which makes use of a commercially available membrane-type surface-stress sensor¹ (MSS), originally intended to function as a gas sensor². The commercial device has piezoresistors embedded in a silicon membrane, upon which a sample can be placed. Piezoresistive materials change in electrical resistivity when mechanical strain is applied. Therefore, torque exerted on the membrane and thus on the piezoresistors causes a change in their resistances. By making a Wheatstone bridge circuit using the piezoresistors on the device, a torque on the membrane results in a voltage across the bridge circuit, which can be used to measure the torque. The goal is to eventually be able to use the new device at low temperature, at high magnetic fields in pulse magnets.

Group Posters/Presentations

Biosciences

Student(s): Lamcaj, Sara; Schambach, Jenna Young

Student Names	University/School	Program	PAD/Group	Mentor
Lamcaj, Sara	Seton Hall University	USG/Postbac	PADSTE/B-11	Barry, Amanda N, B-11
Schambach, Jenna Young	University of Delaware	Post Masters	PADSTE/B-11	Barry, Amanda N, B-11

Category: Biosciences

Type: Group Poster

LA-UR: LA-UR-18-25455

Investigating the lignocellulosic degradation activity of Auxenochlorella Protothecoides

Advancing efforts in renewable energy is of national importance and provides possible solutions to priorities for the United States including reducing carbon emissions and decreasing dependence on foreign oil. Algae have a substantial capability to support the biofuel industry due to their ability to produce refinery-compatible jet fuel precursors. A recently discovered mixotrophic green algae *Auxenochlorella protothecoides* show tremendous effort to support the biofuel industry due to the potential of this algae to degrade complex lignocellulosic material. This degradation is significant because plant substrates can be utilized to massively increase algal biomass and lipid composition, the precursors to jet fuel. Five potential proteins have been identified in the algae that are upregulated transcriptionally in the presence of plant substrate. The main goal of this work was the following: to express, purify and characterize these potential cellulases and to examine the increase in algal biomass productivity due to plant substrate addition.

Computing

Student(s): Akhmetova, Dana; Lakshmiranganatha, Sumathi; Mukherjee, Diptajyoti; Ouellet, Frederick; Payne, Patrick Charles; Stegmeier, Nicholas William

Student Names	University/School	Program	PAD/Group	Mentor
Akhmetova, Dana	KTH Royal Institute of Technology (Sweden)	GRA	PADSTE/CCS-7	Junghans, Christoph, CCS-7
Lakshmiranganatha, Sumathi	University of Wyoming	GRA	PADSTE/CCS-7	Junghans, Christoph, CCS-7
Mukherjee, Diptajyoti	Allegheny College	GRA	PADSTE/CCS-7	Junghans, Christoph, CCS-7
Ouellet, Frederick	University of Florida	GRA	PADSTE/CCS-7	Junghans, Christoph, CCS-7
Payne, Patrick Charles	Stony Brook University	USG/Postbac	PADSTE/CCS-7	Junghans, Christoph, CCS-7
Stegmeier, Nicholas William	South Dakota State University	GRA	PADSTE/CCS-7	Junghans, Christoph, CCS-7

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-26083

Performance Study and Optimization of FleCSALE using Tabular Equation of State

FleCSALE is a software package developed for studying continuum dynamics problems, such as fluid flow. It is specifically developed for existing and emerging large distributed memory system architectures. These emerging high performance computing (HPC) platforms will likely have varied levels of heterogeneity. As such, reaching peak performance will require combined distributed and shared memory models, such as MPI+OpenMP, with full awareness of hardware aspects like memory locality and compute and message passing concurrency. To accommodate future hardware architectures, FleCSALE is built on FleCSI, the Flexible Computational Science Infrastructure, which is designed to allow flexibility in choosing runtime implementations and optimizations. The goal of this research was to increase the performance of FleCSALE, particularly in the context of tabular equation of state (EOS) through the EOSPAC library. As a starting point, the code was refactored to incorporate batch processing of EOSPAC interpolation calls, and memory access optimizations to the sparse data structure used in FleCSALE were studied. By batching the interpolation calls and exploring performance improvements in EOSPAC source code, we were able to take better advantage of on-node parallelism. With the goal of performance portability and exploiting the heterogeneity of future machines, we investigate models like OpenMP, CUDA, and Thrust to accelerate the interpolation routines native to EOSPAC and the fluid dynamics computations in FleCSALE. We compare the performance of these strategies with MPI and Legion as distributed memory backends.

Student(s): An, Cheng; Chen, Charlie

Student Names	University/School	Program	PAD/Group	Mentor
An, Cheng	Texas A&M University	GRA	PADSTE/NSEC	Pawar, Rajesh J, EES-16
Chen, Charlie	Purdue University	USG/Postbac	PADSTE/NSEC	Pawar, Rajesh J, EES-16

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-26021

Parallelize Subsurface Flow Simulator using a Hybrid MPI-OpenMP-GPU Approach

The Finite Element Heat and Mass Transfer Code (FEHM) has been widely used for a variety of subsurface problems, such as CO₂ sequestration, nuclear waste isolation, and oil and gas flow simulation. However, the more expensive computational efforts and longer computational time become a challenge for large, more realistic reservoir models. By taking advantage of the combined distributed and shared memory architectures, the objective of this study is to parallelize the FEHM for significantly reducing the computational time and improving the simulation performance of larger and more complicated problems. The scalable PETSc solver is implemented into the original code, where both MPI and GPU are used to parallelize the matrix calculation. Meanwhile, OpenMP and vectorization are applied for the large-loop computation. The benefits and difficulties of each parallelization approach are evaluated as well.

Student(s): Carrillo Cabada, Hector Alexis; Kim, Heesoo

Student Names	University/School	Program	PAD/Group	Mentor
Carrillo Cabada, Hector Alexis	University of New Mexico	USG/Postbac	PADSTE/NSEC	Haack, Jeffrey Robert, CCS-2
Kim, Heesoo	Brown University	USG/Postbac	PADSTE/NSEC	Haack, Jeffrey Robert, CCS-2

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-26036

Parallel and on-the-fly weight computation for the Boltzmann transport equation

The numerical simulation of the Boltzmann Transport Equation (BTE) is of interest to many applications because the equation models the properties and behaviors of dilute gases or plasmas as the particles undergo collisions. In particular, the BTE describes the time evolution of the probability density function of finding gas particles at a particular location with a particular velocity at a given time. The time evolution of the distribution function is calculated by solving a 5D integral at each point in a 3D velocity space, which can be simplified into a 3D integral via taking a Fourier transform. However, on taking the Fourier transform, the equation gains a constant 6D convolutional weights, with a single weight per 3D velocity pair. These weights must either be stored on node during computation (which is not realistic for large scale computations), or recalculated at every time step. In this presentation, we explore both options by distributing weights across several nodes using MPI and by recalculating the weights on the fly at every time step on GPU using CUDA.

Student(s): Duarte, Marco Antonio; Everson, Kody Jacob; Rindels, Raymond Luke

Student Names	University/School	Program	PAD/Group	Mentor
Duarte, Marco Antonio	University of North Texas	USG/Postbac	PADSTE/HPC-ENV	Lopatina, Lena, HPC-ENV
Everson, Kody Jacob	Dakota State University		PADSTE/HPC-ENV	Lopatina, Lena, HPC-ENV
Rindels, Raymond Luke	New Mexico Tech	USG/Postbac	PADSTE/HPC-ENV	Lopatina, Lena, HPC-ENV

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-26251

User-Accessible Cluster Monitoring

Los Alamos National Laboratory has been at the frontier of science and supercomputing since it opened its doors in 1943. Many scientists at Los Alamos use massively parallelized networks of computers called clusters or High Performance Computers (HPC) to perform work relevant to basic science and national security. As problems get larger and more complex, the High Performance Computing division strives to provide corresponding state of the art computing resources. LANL has thousands of users utilizing computing capabilities simultaneously. One challenge for users of HPC systems is keeping up with the status and availability of those shared resources to maximize throughput and performance. As of now, it is not possible for users to see system metrics that might explain variability in performance. For example, large amounts of storage access by one user can affect the performance of other users' applications. If such real time knowledge is available, users can switch to alternative storage and speed up their work. Real time system metrics can also improve scheduling of resources by the system to maximize total throughput. Additionally, performance predictability is important to maintain the cluster's schedules and to help plan for hardware upgrades in the future. Obtaining, storing, analyzing, and displaying system metrics requires overcoming a lot of technical challenges, such as computational overhead, non-locality of the data, and presenting large amounts of data in a manner that is easy to understand. To address this problem, we developed and implemented a method of obtaining and aggregating system metrics. We set up various monitoring tools for different metrics of interest, found a way to aggregate the obtained data in a shared database, and developed a way to present the systems' metrics in an intuitive way to the user. This allows for a quick overview of cluster performance.

Student(s): Dubey, Mohit Lauer; Jones, Haydn Thomas

Student Names	University/School	Program	PAD/Group	Mentor
Dubey, Mohit Lauer	Oberlin College and Conservatory	USG/Postbac	PADSTE/NSEC	Kenyon, Garrett, CCS-3
Jones, Haydn Thomas	New Mexico Institute of Mining and Technology	USG/Postbac	PADSTE/NSEC	Kenyon, Garrett, CCS-3

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-25994

Versatile Scaling for Neurally Inspired Auditory Source Separation

The human auditory cortex is a massively parallel and efficient encoding system that solves difficult signal processing problems, such as the separation of multiple independent sources from a single waveform with ease. Despite recent advances in computation the auditory cortex has yet to be modeled at scale to solve this blind source separation problem. To address the computational demands we investigate scalability of different problem sizes using batching and meshing techniques. Using the neural simulation toolbox PetaVision on a heterogenous, multi-node cluster, we model the primary auditory cortex at scale to separate multiple instruments from musical tracks.

Student(s): Gafur, Jamil; Kempfert, Katherine Candice

Student Names	University/School	Program	PAD/Group	Mentor
Gafur, Jamil	CUNY Lehman College	USG/Postbac	PADSTE/NSEC	Fairchild, Geoffrey, A-1
Kempfert, Katherine Candice	University of Florida	USG/Postbac	PADSTE/NSEC	Manore, Carrie Anna, T-6

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-25999

Forecasting Dengue in Brazil with Time Series Modeling in Parallel

Early detection of diseases outbreaks is instrumental in reducing mortality and other costs. However, predictive systems for diseases with strong environmental drivers have been underutilized. To address this need, we develop a scalable workflow that integrates large, diverse data sources to predict disease at various spatiotemporal resolutions. Fitting thousands of time series models in parallel, interpretation of the model ensemble can improve understanding of the disease and inform public health policy. Our approach is applied to Brazil's outbreak of dengue, a mosquito-borne virus that infects more than one million people a year and strains public health and the economy. Seasonal components of dengue are captured by combining demographic information with time series from nontraditional sources (e.g., Google search trends and satellite images). With low testing error, memory usage, and runtime, our approach enables effective real-time forecasting to target outbreaks as they occur.

Student(s): Goetsch, Timothy Tyler; Haque, Abida

Student Names	University/School	Program	PAD/Group	Mentor
Goetsch, Timothy Tyler	New Mexico Institute of Mining and Technology	USG/Postbac	PADSTE/NSEC	Nam, Hai Ah, CCS-2
Haque, Abida	North Carolina State University	GRA	PADSTE/HPC-DES	Monroe, Laura Marie, HPC-DES

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-25835

Budget Aware Computation: Affordable Precision on Mini-Apps

Current architectures promote the use of 64-bit precision because it has little cost difference from 32-bit precision and has higher numerical fidelity. However, future architecture is trending towards more native lower precision operations. We use reduced floating point precision and higher resolution in high performance scientific computations, and therefore improve solution fidelity for a fixed computational budget. Finally, we describe the trade-offs between storage costs, energy, and runtime across different levels of floating point precision.

Student(s): Harrell, Stephen Lien; Kitson, Joy

Student Names	University/School	Program	PAD/Group	Mentor
Harrell, Stephen Lien	Purdue University	GRA	PADSTE/NSEC	Bird, Bob, CCS-7
Kitson, Joy	University of Delaware	USG/Postbac	PADSTE/NSEC	Bird, Bob, CCS-7

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-25930

Plasma Meets Portability: A journey to performance portability in a physics code

In our journey to exascale, it is imperative that applications not only run efficiently, but do so on a wide variety of platforms at a reasonable cost. The Vector Particle in Cell (VPIC) application is a plasma physics code that is highly performant, but past efforts to make it more portable have come at a heavy maintenance cost. In order to alleviate this cost, we leverage a portability framework called Kokkos to maximize both the code shared between platforms and the performance of the application. In the process, we develop metrics of developer productivity, which can be used to holistically assess how productively performance portable (PPP) an application is.

Student(s): Hsu, Abigail Elaine; Neill, David Howard

Student Names	University/School	Program	PAD/Group	Mentor
Hsu, Abigail Elaine	Stony Brook University	USG/Postbac	PADSTE/NSEC	Carlson, Neil, CCS-2
Neill, David Howard	Grinnell College	USG/Postbac	PADSTE/NSEC	Carlson, Neil, CCS-2

Category: Computing

Type: Group Poster

LA-UR: LA-UR-18-26037

Challenges of Performance Portability for Fortran Unstructured Mesh Codes

This project investigates how different approaches to parallel optimization impact the performance portability for unstructured mesh codes. In addition, we explore the productivity challenges of improving performance of a Fortran codebase. For this study we build upon the Truchas software, a castin manufacturing simulation code, and develop initial ports for pure OpenMP, MPI+OpenMP, and MPI+CUDA for three key computational kernels.

Earth & Space Sciences

Student(s): An, Cheng; Chen, Charlie

Student Names	University/School	Program	PAD/Group	Mentor
An, Cheng	Texas A&M University	GRA	PADSTE/NSEC	Pawar, Rajesh J, EES-16
Chen, Charlie	Purdue University	USG/Postbac	PADSTE/NSEC	Pawar, Rajesh J, EES-16

Category: Earth & Space Sciences

Type: Group Poster

LA-UR: LA-UR-18-26021

Parallelize Subsurface Flow Simulator using a Hybrid MPI-OpenMP-GPU Approach

The Finite Element Heat and Mass Transfer Code (FEHM) has been widely used for a variety of subsurface problems, such as CO₂ sequestration, nuclear waste isolation, and oil and gas flow simulation. However, the more expensive computational efforts and longer computational time become a challenge for large, more realistic reservoir models. By taking advantage of the combined distributed and shared memory architectures, the objective of this study is to parallelize the FEHM for significantly reducing the computational time and improving the simulation performance of larger and more complicated problems. The scalable PETSc solver is implemented into the original code, where both MPI and GPU are used to parallelize the matrix calculation. Meanwhile, OpenMP and vectorization are applied for the large-loop computation. The benefits and difficulties of each parallelization approach are evaluated as well.

Engineering

Student(s): Brand, Howard James; Kauppila, Tia Morgaine; Wielgus, Kayla Marie

Student Names	University/School	Program	PAD/Group	Mentor
Brand, Howard James	Clemson University	GRA	PADSTE/NSEC	Mascarenas, David Dennis Lee, NSEC
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Category: Engineering

Type: Group Poster

LA-UR: LA-UR-18-25856

Imager-based Characterization of Viscoelastic Material Properties

In this work we explore the use of emerging full-field, high-resolution, modal identification techniques from video to characterize viscoelastic material properties. Currently, there are no cost-effective methods to directly measure viscoelastic material properties at intermediate strain rates. These properties can be measured at low strain rates using quasi-static loading techniques, while Split-Hopkinson's bar tests are used at high strain rates. Determining material properties at the intermediate strain rate regime is challenging as it requires large, expensive testing apparatuses and involves complex experimental protocols. An imager-based technique would provide a simpler, more affordable method for measuring viscoelastic material properties at these strain rates. To obtain measurements for intermediate strain rates of viscoelastic materials, we develop a testing protocol that involves creating a simple structure from the material-under-test and measuring its vibrational response using an imager. A finite-element model of the viscoelastic testing structure is also constructed. We extract full-field, high resolution modal shapes and coordinates from the video measurements of the structure's vibrations in the desired strain regime. The frequencies of oscillation and the damping ratios are then identified. This information is us

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Category: Engineering

Type: Group Poster

LA-UR: LA-UR-18-25857

Augmented Reality for Enabling Smart Nuclear Infrastructure at LANL

There is a high interest in improving the criticality safety and operational capabilities of nuclear facilities with augmented reality. To do so, we must achieve four primary objectives: automated material move planning, smart cart localization, integration of thermal imager, and documentation accessibility. Because safety is of utmost importance especially when working in a hazardous environment such as a nuclear facility, automated material move planning is crucial in guaranteeing the safest path to transport material from one location to another taking into consideration the location of gloveboxes, nuclear criticality limits associated with each glovebox, and the chemical properties associated with the material being transported. Since items can easily be lost or misplaced, it is important to assign each with a QR code such that we can identify its location. Furthermore, it is quintessential to implement a 3D model of a nuclear facility for smart cart localization to track the movements of all people and items. The process of transporting material requires the operator wearing an AR headset to authenticate himself, scan the QR code of the material, and scan the NFC tag reader on the smart cart to prepare for transfer. For further safety regulations, the integration of a thermal imager onto the AR headset would warn the operator if there is a potential danger and alert nearby coworkers in the vicinity. The abilities to access documentation and interface with the database are essential in the organization and structure of a nuclear facility. Submitting and retrieving information through an AR headset is not only user-friendly, but also systematic in terms of networking. Augmented reality presents a promising path that paves a way for a safer and better work environment in nuclear facilities.

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Category: Engineering

Type: Group Poster

LA-UR: LA-UR-18-25869

Imager-based Techniques for Analyzing Metallic Melt Pools for Additive Manufacturing

We present the development of new vision-based algorithms for extracting physical properties, such as depth, from melt pools. Having a consistent and appropriately-sized pool is critical to a strong weld and producing high quality metallic additively manufactured parts. Melt pool depth is an important variable to observe; but, currently, there are no techniques for quantitatively characterizing melt pools remotely. The bandwidth requirements for traditional high speed video is too high for real time analysis. Silicon retinas are event-based imagers that record individual pixel's changes in intensity over time. This method of imaging has a very fine temporal resolution, high dynamic range, and low bandwidth requirement. These properties, alongside the cost efficient hardware, make real time online monitoring of additive manufacturing and laser welding possible. Furthermore, the ability to monitor melt pools in real time could improve the quality of laser printed parts and welds because it would allow automatic control systems to recognize and correct imperfections during the printing and welding processes. By measuring the oscillations of a melt pool with a silicon retina then applying a principal component analysis and a complexity pursuit algorithm, we will be able to determine the modes of the pool and correlate the natural frequencies and pool geometry. Measurements are compared with a finite element model of the melt pool.

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Student Names	University/School	Program	PAD/Group	Mentor
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Category: Engineering

Type: Group Poster

LA-UR: LA-UR-18-26400

Engineering the Universal Bacteria Sensor

There is a high interest in improving the criticality safety and operational capabilities of nuclear facilities with augmented reality. To do so, we must achieve four primary objectives: automated material move planning, smart cart localization, integration of thermal imager, and documentation accessibility. Because safety is of utmost importance especially when working in a hazardous environment such as a nuclear facility, automated material move planning is crucial in guaranteeing the safest path to transport material from one location to another taking into consideration the location of gloveboxes, nuclear criticality limits associated with each glovebox, and the chemical properties associated with the material being transported. Since items can easily be lost or misplaced, it is important to assign each with a QR code such that we can identify its location. Furthermore, it is quintessential to implement a 3D model of a nuclear facility for smart cart localization to track the movements of all people and items. The process of transporting material requires the operator wearing an AR headset to authenticate himself, scan the QR code of the material, and scan the NFC tag reader on the smart cart to prepare for transfer. For further safety regulations, the integration of a thermal imager onto the AR headset would warn the operator if there is a potential danger and alert nearby coworkers in the vicinity. The abilities to access documentation and interface with the database are essential in the organization and structure of a nuclear facility. Submitting and retrieving information through an AR headset is not only user-friendly, but also systematic in terms of networking. Augmented reality presents a promising path that paves a way for a safer and better work environment in nuclear facilities.

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Potts, Dewey	Brigham Young University	USG/Postbac	PADSTE/LADSS	Cattaneo, Alessandro, AET-1

Category: Engineering

Type: Group Poster

LA-UR: LA-UR-18-25385

Augmented Reality for Interactive Robot Control

Robots are widely used to support mission-critical, high-risk and complex operations. Human supervision and remote robot control is often required to operate in these scenarios. In order to improve the usability of robots, we propose utilizing augmented reality (AR) as a novel solution for controlling robots which is more intuitive and less training intensive than traditional joystick control. AR technology can interpret a physical motion and turn it into a robot-command as well as project a hologram into the user's view. These abilities make robotic control more intuitive because inputs involve already familiar body movements and holographic outputs imitate real world objects. In our project, a Microsoft HoloLens headset is used as the AR component. At a high level, the HoloLens is the bridge between what the user sees/does, the control of the robot, and a holographic user interface. First, the cameras from the HoloLens create a geometric mesh of the environment which is sent to the main robotic application (ROS libraries) which performs the robot's motion planning. Second, the user indicates a robotic command with a hand gesture which is sent to ROS. Third, ROS creates a motion plan to implement the user command while taking into account the geometry of the environment to avoid collisions.

Information Technology

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Category: Information Technology

Type: Group Poster

LA-UR: LA-UR-18-25831

Creating a Multi-Model of Alzheimer's Disease Patients to improve Early Detection **Methods**

An estimated 50 million people were living with dementia in 2017, and the majority are thought to have Alzheimer's disease. Alzheimer's is not only one of the top 10 leading causes of death in high income countries, but is also the only of those diseases that cannot be prevented, slowed, or cured. For these reasons, there is a call to research the disease and improve our ability to recognize the disease before it progresses into later stages that are untreatable. There is hope that starting treatments for the disease before the onset of symptoms can lead to improved quality of life for the patient later on, and can greatly slow the progression of the disease. We propose to use deep sparse coding methods to learn discriminative multi-modal features combining brain-labeling data, fMRI/ MRI, cognitive assessments, and biometrics for the early detection of Alzheimer's disease. We will test the hypothesis that by combining multiple measurement modalities, we will be able to construct more predictive features than would be possible from consideration of each modality separately.

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Category: Information Technology

Type: Group Poster

LA-UR: LA-UR-18-26437

Exploring Thrill: A Distributed Big Data Analytics Framework for HPC and Cloud Platforms

There are two major methods to provide scalable distributed data analysis. Frameworks like Spark work on Cloud platforms. They are built upon Scalar/Java with TCP. It is easy to program with such frameworks. On the other hand, handcrafted C/C++ data processing algorithms with MPI work on HPC platforms. They have high performances. The Thrill library (Bingmann, 2016) is designed to combine the advantages from the above two approaches. It provides a high-level application programming interface (API) similar to Apache Spark while taking advantage of the high performance of the C++ programming language and MPI communication. Project Tivra explores the use of Thrill to help scientists in data analysis at LANL. In the first stage, we implemented the same functionalities with Thrill to analyze cosmology data from HACC (Salman, 2016) as SQLite queries. We conducted scalability tests of our implementations. In the second stage, we worked with Dr.Fan Guo and Dr.Xiaocan Li from the VPIC to implement sorting for data analytic and plotting particle trajectories. We also worked with Dr.Danny Perez from the accelerated molecular dynamics (AMD) open science simulations to extract features from MD simulation and we went further in time series plotting and states clustering analytics. We implemented the above data analytic operations requested by scientists using Thrill and measured the performance and scalability of the applied data analytic operations using LANL's cluster resources. For the completeness of the research, we conducted similar scalability experiments on Amazon Web Service (AWS) to demonstrate that the library supports both platforms and to understand and compare the performance characteristics of these two platforms. The above analysis helped us to explore a potential path to transit LANL's scientific computation to the Cloud.

Materials Science

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Category: Materials Science

Type: Group Poster

LA-UR: LA-UR-18-25638

Shock Experiments on Additively Manufactured and Wrought Tantalum

For thousands of years, metals have been made with the same basic principles. These processing principles are understood, hence the behavior of the resulting material can be predicted with confidence. During additive manufacturing (AM), those principles are altered and create a product with a novel microstructure. Due to the nascent stage of additive manufacturing, the microstructure varies greatly with build parameters, which causes a variation in the performance of the material. Understanding the influence of the varying microstructure on the performance of metals can help develop a model to understand AM material behavior. In these experiments, samples from both a wrought tantalum plate and a build of AM tantalum were shocked with a single stage, 80mm gas gun. Photonic Doppler Velocimetry (PDV) was deployed to record the free surface velocity of each sample. The samples were soft recovered, sectioned, and imaged to view the voids formed from impact. The AM sample had a columnar microstructure in the build direction, while the wrought tantalum expressed an equiaxial microstructure. Due to the different microstructures, the damage in each sample varied. Impurities introduced during the AM process acted as void nucleation sites in the sample. The results showed that the AM sample behaved less ductile than the wrought tantalum sample. The AM sample had a higher compressive strength, but a lower tensile strength than the wrought sample. These experiments highlight the importance of high rate material testing and give us a better understanding of how various materials react when subjected to extreme dynamic conditions.