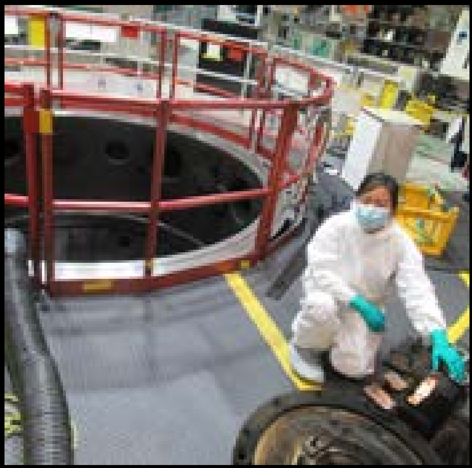
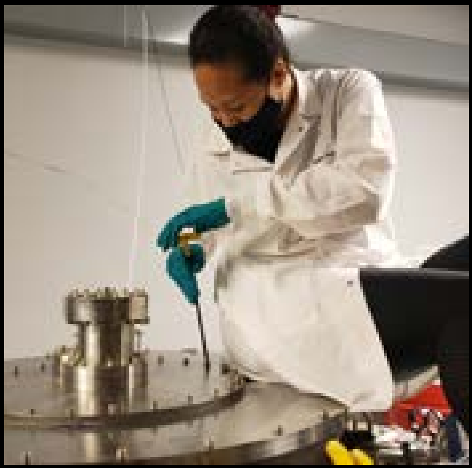
DOE/NA-0113

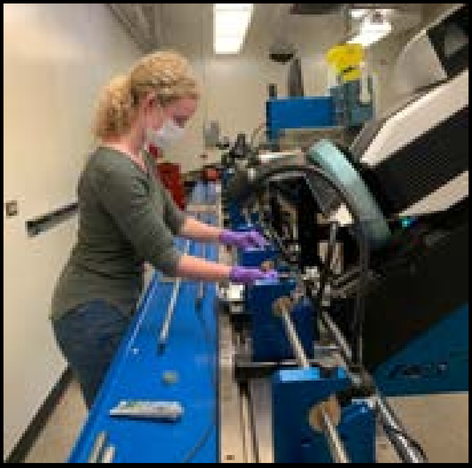
2021 Academic Programs Annual

Office of Research, Development, Test, and Evaluation

- Stewardship Science Academic Alliances
- High Energy Density Laboratory Plasmas
- National Laser Users' Facility
- Predictive Science Academic Alliance Program III
- Minority Serving Institutions Partnership Program
- Fellowship Programs



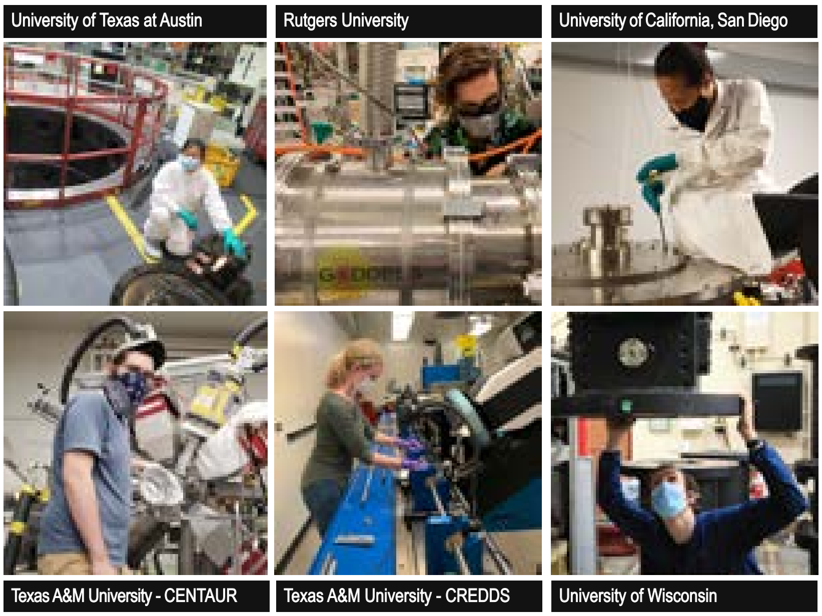





NNSA National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY

On the Cover



The COVID-19 pandemic changed the face of research for the Department of Energy/ National Nuclear Security Administration's Academic Programs during 2020.

— Images courtesy of the following DOE/NNSA academic partners: (top row, L-R) University of Texas at Austin, Rutgers University, University of California, San Diego, (bottom row) Texas A&M University, and the University of Wisconsin

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National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY

2021
Academic Programs Annual

NNSA Office of Research, Development, Test, and Evaluation

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NNSA
National Nuclear Security Administration

"Training and recruiting the next generation of nuclear security stewards is the primary goal of our academic programs, ensuring the quality of our workforce and the nuclear deterrent."

— Dr. Mark C. Anderson
Assistant Deputy Administrator
for Research, Development, Test, and Evaluation

✦ ✦ ✦

Welcome from the Assistant Deputy Administrator for Research, Development, Test, and Evaluation

There are many great parts to my job. One of them, and one that I look forward to each year, is the opportunity to communicate with you—the next generation of nuclear security stewards. Communication is particularly challenging, as we continue to face the isolation imposed by the global COVID-19 pandemic. Nevertheless, we continue to execute the primary mission of the National Nuclear Security Administration (NNSA) of ensuring a safe, secure, and effective nuclear deterrent in the absence of nuclear testing. With the innovation of our staff and by embracing evolving technologies, we are able to meet as a community virtually this year and host the Stewardship Science Academic Programs Symposium on-line. What a challenge and what a wonderful opportunity for us all to come together in these challenging times.

As we are approaching nearly 30 years of conducting the nuclear weapons program without needing to perform underground nuclear weapons testing, we remain diligently focused on our mission and are grateful for the many former participants from our Academic Programs who have chosen a career with the NNSA national laboratories. Everyday we have evidence that our efforts are keeping the Unites States, its allies, other friends, and the world-at-large safe through nuclear deterrence.

Nuclear deterrence has been shown to work, but deterrence needs continued strengthening to ensure continued success. World-class, state-of-the-art science and technology is the key ingredient that we have as a nation to maintain the effectiveness of our nuclear deterrent. Training and recruiting the next generation of nuclear security stewards is the primary goal of our academic programs, ensuring the quality of our workforce and the nuclear deterrent.

The value of the work and the people contributing to build a safer world is evident in the pages of this Academic Programs Annual. We feature select students pursuing doctoral degrees and alumni of the Academic Programs who write in their own words about their perspective on the Academic Programs and the opportunities that it has afforded them. We are honored to have all of you as part of our team, and to you I extend my congratulations for your successes to date and for your continued success in the future.

Dr. Mark C. Anderson

Assistant Deputy Administrator
for Research, Development, Test, and Evaluation
National Nuclear Security Administration

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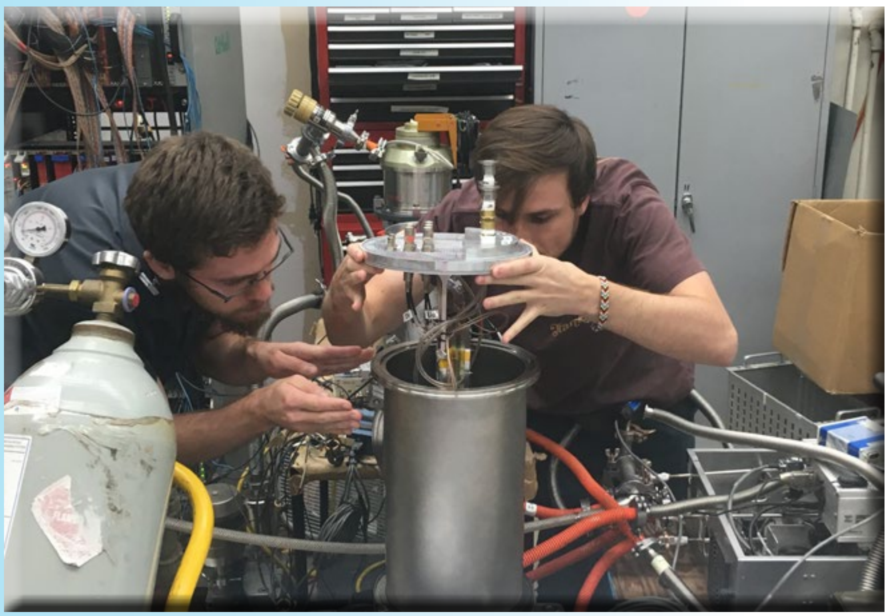
Outstanding Poster Awards

2020 Stewardship Science Academic Programs Symposium

Almost 120 graduate student posters were featured at the 2020 Stewardship Science Academic Programs Symposium. Pictured above, from left to right, are Ann J. Satsangi, SSAA Program Director; Outstanding Poster Award recipients Shu Zhang, Ashley Williams, Rebecca Toomey, Maren Hatch, Daniel Felton, Paul Fanto, Benjamin Brugman, and David Bernstein; and Michael Kreisler, Science Advisor to NNSA.



Overview

Academic Programs

Office of Research, Development, Test, and Evaluation

— Training the Next Generation of Stockpile Stewards

The challenges of modernizing our nuclear stockpile demand a strong and diverse base of national expertise and educational opportunities in specialized technical areas that uniquely contribute to nuclear stockpile stewardship. The Academic Programs of the National Nuclear Security Administration (NNSA) Office of Research, Development, Test, and Evaluation (RDT&E) are designed to support academic programs in science and engineering disciplines of critical importance to the Nuclear Security Enterprise (NSE), such as nuclear science, radiochemistry, materials at extreme conditions, high energy density science, advanced manufacturing, and high performance computing. In addition, building a diverse workforce will strengthen our stewardship of the future. The role of the Academic Programs is three-fold:

- Develop the next generation of highly-trained technical workers able to support its core mission
- Maintain technical peer expertise external to the NSE for providing valuable oversight, cross-check, and review
- Enable scientific innovation to enhance the NSE missions to strengthen the basic fields of research relevant to the NNSA mission.

Imperial College PhD student Vicente Valenzuela-Villaseca making adjustments to an X-ray framing camera used to study rotating plasma flows on the MAGPIE pulsed power machine.

The Academic Programs enable a robust and diverse research and science, technology, engineering, and mathematics (STEM) educational community through a variety of methods of support. Investments in consortia and centers of excellence provide collaborative groups to tackle large questions through multi-disciplinary approaches and leverage preeminent scientists in the field. Research grants and Focused Investigatory Centers support individual principal investigators to foster a vibrant community responsive to new breakthroughs by providing flexibility for new ideas, diversity, and career growth. Specific support to minority and tribal serving institutions prepares a diverse workforce of world-class talent through strategic partnerships. Fellowships provide graduate students with key opportunities to connect with the Department of Energy/ National Nuclear Security Administration (DOE/NNSA) missions and to provide direct experiences at the Nuclear Security Enterprise (NSE) sites. User Facilities open opportunities for academic partners to use NNSA's cutting edge research facilities and to push frontiers of current scientific understanding. Several underlying features of all Academic Programs include the focus on quality science through competitive award, connection with NNSA mission lab/site work, and a view to future needs and opportunities of the NSE.

The Academic Programs is comprised of five subprograms:

- ✦ Stewardship Science Academic Alliances;
- ✦ High Energy Density Laboratory Plasmas;
- ✦ Predictive Science Academic Alliance Program;
- ✦ Minority Serving Institutions Partnership Program; and
- ✦ Fellowship Programs.

Stewardship Science Academic Alliances

The Stewardship Science Academic Alliances (SSAA) Program supports scientific academic research programs to develop the next generation of highly trained, technical workers able to support its core mission and to ensure there is a strong community of technical peers, external to the NNSA national laboratories, capable of providing peer review and scientific competition to strengthen the basic fields of research relevant to the NSE.

Minority Serving Institutions Partnership Program

The SSAA Program funds both collaborative Centers of Excellence and smaller individual investigator research projects to conduct fundamental science and technology research of relevance to stockpile stewardship. Current technical areas include studies of materials under extreme conditions, low-energy nuclear science, high energy density physics, and radiochemistry. SSAA funding supports research at approximately 80 universities, including training of over 350 undergraduate students, graduate students, and postdoctoral researchers each year. A key element of both centers of excellence and individual investigator awards is the connection of students with the NSE. These opportunities are focused in technical fields critical to stewardship science and build a field of talented researchers and committed doctoral students sharing a common desire to advance science while impacting national security.

Minority Serving Institutions Partnership Program

The NNSA Minority Serving Institutions Partnership Program (MSIPP) mission is to create and foster a sustainable STEM pipeline that prepares a diverse workforce of world-class talent through strategic partnerships between Minority Serving Institutions and the NSE. MSIPP supports Historically Black Colleges and Universities (HBCUs), Hispanic Serving Institutions (HSIs), and Tribal Colleges and Universities (TCUs). MSIPP aligns investments in university capacity and workforce development with the NNSA mission to develop the needed skills and talent for the NSE’s enduring technical workforce and to enhance research and educational capacity at under-represented colleges and universities.

This alignment is defined by the following goals:

1. Strengthen and expand minority and tribal serving institutions’ educational and/or research capacity in NNSA mission areas of interest.
2. Target collaborations between minority and tribal serving institutions and the NSE that increase interactions to provide minority and tribal serving institutions direct access to NSE resources.
3. Increase the number of MSI students who graduate with STEM degrees relevant to NNSA mission areas and who have had exposure to career opportunities within the NSE.
4. Increase the number of minority graduates and postdoctoral students hired into the NSE’s technical and scientific workforce.

High Energy Density Laboratory Plasmas

High energy density (HED) science is central to many aspects of nuclear weapons, and maintaining a strong HED academic community in this unique field will be critical for the future needs of a modern nuclear stockpile. The Joint Program in High Energy Density Laboratory Plasmas (JPHEDLP) is designed to steward the study of laboratory HED plasma physics by funding academic research of ionized matter in laboratory experiments where the stored energy reaches approximately 100 billion joules per cubic meter (i.e., pressures of approximately 1 million atmospheres). The program supports three primary elements: individual investigator research grants, centers of excellence, and the National Laser Users' Facility.

Various workshops, training, and recruitment events are organized by the High Pressure Collaborative Access Team, a dedicated facility for experimental research on materials under extreme pressure-temperature conditions. Photo was taken during the January 2020 "Introduction to Technique and Capabilities at HPCAT" workshop.

Individual Investigator Grants

NNSA's Office of Experimental Sciences partners with the DOE's Office of Fusion Energy Sciences to issue an annual joint solicitation for HEDLP research. The coordination across agencies enables the support of a strong and broad academic presence in HED science, leveraging common interests and assuring NNSA-specific interests in this area remain vibrant. Competitively awarded research grants are selected through the joint solicitation conducted in coordination with the Office of Science.

Centers of Excellence

The Joint Program in HEDLP provides funding support toward the HED Centers of Excellence selected under the competitive SSAA Centers process. Centers of Excellence are an integrated, multi-institutional, collaborative effort focused on a central problem or theme. These Centers work closely with NSE scientists and maintain a core set of academic expertise in key technical areas.

National Laser User Facility (NLUF)

The primary purpose of the NLUF program is to provide facility time access to NNSA-unique tools to accomplish cutting edge science. In the pursuit of fundamental science advances, the innovative development of diagnostics and platforms by user facility partners often have proven to benefit NNSA experimental needs. Hands-on research experience is provided to academic and industrial researchers using the OMEGA and OMEGA EP facilities as tools for conducting basic research experiments.

> *"The Academic Programs of the NNSA's Office of Research, Development, Test and Evaluation are designed to support academic programs in science and engineering disciplines of critical importance to the Nuclear Security Enterprise (NSE), such as nuclear science, radiochemistry, materials at extreme conditions, high energy density science, advanced manufacturing, and high performance computing."*

Predictive Science Academic Alliance Program

The Predictive Science Academic Alliance Program (PSAAP) consists of participation by leading U.S. universities, focusing on the development and demonstration of technologies and methodologies to support effective, high performance computing in the context of science and engineering applications. The research performed by the universities in this program is discipline-focused to further predictive science and is enabled by effective extreme scale computing. The predictive science that is a highlight of this program is based on verification and validation and uncertainty quantification for large-scale simulations.

PSAAP has a long-term goal to cultivate the next generation of scientists and engineers to support the Advanced Simulation and Computing and Directed Stockpile Work missions. These efforts establish academic programs for multidisciplinary simulation science and provide students the relevant experience for weapons code development through open science applications.

DOE/NNSA Fellowship Programs

The Academic Programs also includes the Stewardship Science Graduate Fellowship (SSGF), Laboratory Residency Graduate Fellowship (LRGF), and Computational Science Graduate Fellowship (CSGF) programs (jointly sponsored with the DOE's Office of Science). These three programs support PhD students in areas of interest to stockpile stewardship. SSGF and CSGF provide a yearly stipend, tuition fees, lab practicums, and an academic allowance. The LRGF program extends those benefits to at least two longer practicums and encourages fellows to pursue their thesis research in collaboration with lab scientists. This Annual highlights a select few alumni and students from each fellowship. For more information about these programs, please visit http://www.krellinst.org/fellowships.

Supporting Research from Different Angles

From Stewardship Science Academic Alliances to the National Nuclear Security Administration

Dr. Rebecca (Becky) Lewis, Federal Program Manager ✦ National Nuclear Security Administration

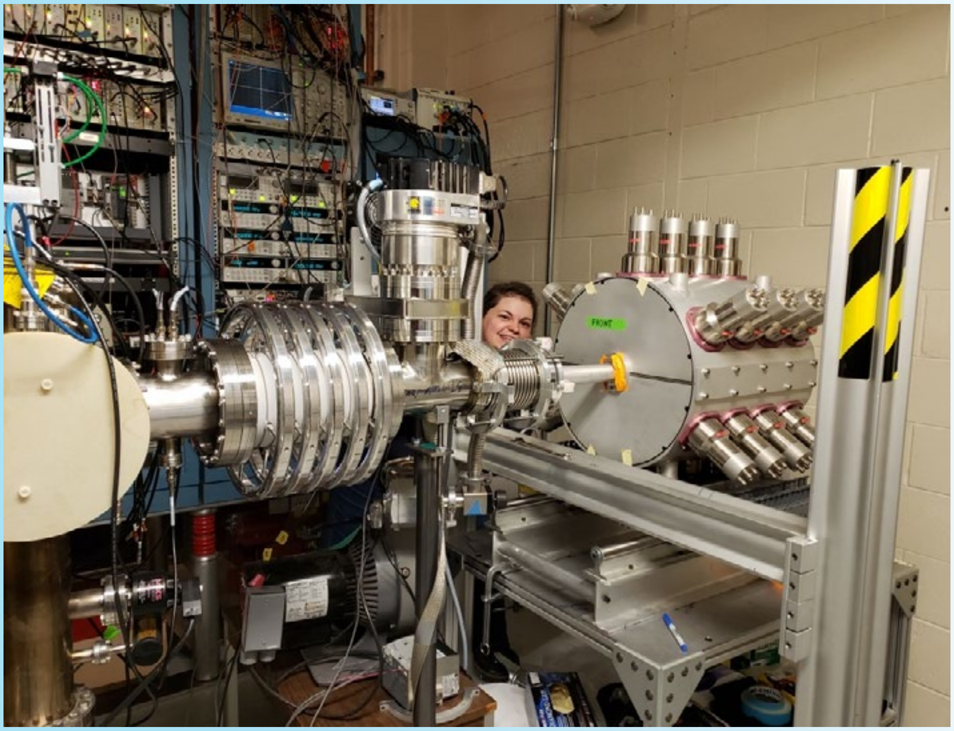
The SSAA program provided Lewis with a variety of invaluable experiences. (a) Lewis received Outstanding Power Awards at the 2018 and 2019 Stewardship Science Academic Programs (SSAP) Symposia. She is pictured with her poster "Experimentally Constrained Neutron-rich Nickel Cross Sections" at the 2019 Symposium. (b) Lewis and former postdoctoral researcher, now beam physicist, Mallory Smith preparing the Summing NaI (SuN) detector for an experiment at NSCL. Both Lewis and Smith were funded by an SSAA grant. (c) Lewis dressed up in safety gear to talk to the public about nuclear science at an NSCL Open House. (d) During her time at Los Alamos National Laboratory, Lewis explored the town and its history as well as worked with staff on research projects. She is pictured standing in between statues of The Manhattan Project's J. Robert Oppenheimer (left) and General Leslie R. Groves, Jr. (right).

I became involved in the Stewardship Science Academic Alliances (SSAA) program as a graduate student in Nuclear Chemistry at the National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University in 2016. My advisor at the NSCL, Dr. Sean Liddick, had received an SSAA grant to support my thesis experiment to infer neutron-capture cross sections of neutron-rich Ni isotopes. The opportunities that became available to me as part of the SSAA community were unexpected and amazingly helpful as I finished graduate school and decided what to do next.

Graduate school is hard, stressful, and can feel overwhelming. I found that getting out into the community, both the scientific one and the public one, kept me excited about my research and about science in general. Being able to talk about your own research is important for every scientist, but I learned that being able to talk about science to a more general audience is just as important. The SSAA program emphasizes that skill in many ways. At the annual SSAP symposia, I would have conversations with other graduate students and researchers from the national laboratories that allowed me to learn about other types of science relevant to national security and to practice how I could highlight the impact of the research I was doing.

The strong ties to the national laboratories through SSAA helped me both to finish my research and to decide what I wanted to do next. I spent a semester at Los Alamos National Laboratory (LANL), funded by the SSAA grant, working with staff scientists on a comparison of codes used to calculate neutron-capture cross sections. Spending a few months at LANL gave me the chance to test drive what my life as a postdoctoral fellow would look like at a national laboratory, and it turned out it wasn't what I wanted. After that realization, I started talking to Federal Program Managers (FPMs) in the NNSA Office of Experimental Sciences (OES) about career options and learned about the NNSA Graduate Fellowship Program (NGFP). I joined the 2019-2020 NGFP class, worked in the Office of Defense Nuclear Nonproliferation Research & Development, and was exposed to the other side of research funding—the decision making process and the cooperation between different offices and agencies. I had another chance at a career test drive, and this time I really liked what I saw.

During my NGFP year, I never lost contact with OES. I had learned so much from my interactions during my years in the SSAA, and I wanted to keep learning about the scope of work being done and what opportunities could be next. Then 2020 came with the COVID-19 pandemic just as I was starting my job search, and it was the connections that I had made within NNSA that allowed me to move forward with job opportunities. After many conversations with OES, I was able to join the office when my fellowship ended. This was the ideal solution to a very strange time for a job search and an even better start to my career.



Lewis setting up the Summing NaI (SuN) detector for an experiment at the NSCL.

My involvement with the SSAA exposed me to many career paths and allowed me to discover which role would be the best fit for me. I was able to interact with multiple facets of the nuclear security enterprise, which shaped my decision to become an advocate for exceptional scientific research within the NNSA.

— Dr. Becky Lewis
Federal Program Manager, OES

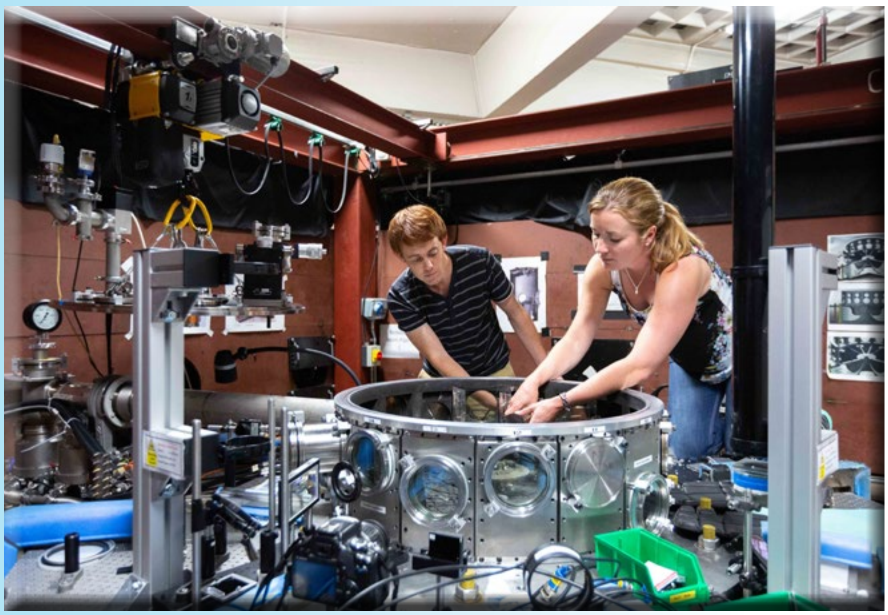
✦ ✦ ✦

I joined OES in June 2020 as the FPM for the Neutron Diagnosed Subcritical Experiments project as well as the federal lead for a comprehensive audit of OES-funded facilities at the national laboratories. The facility audit process has been especially useful for getting exposure to the full range of the research that the office supports and has allowed me to meet people across the complex and to make extremely valuable connections. The transition from doing research to supporting research has been interesting, challenging at times, and completely worth it for me. Talking to as many people as I can, from different organizations and career paths, has helped me decide what I want to be doing and has opened up possibilities that I never would have guessed existed.

Lewis Academic Programs Highlights

Stewardship Science Academic Alliances and the NNSA Graduate Fellowship Program

- Invited to present SSAA-funded research results to the European nuclear physics community at the University of Oslo and at the Russbach School on Nuclear Astrophysics in Austria
- Mentored graduate, undergraduate, and high school students on topics such as experimental design, data analysis, outreach efforts, and career planning
- Presented results of SSAA-funded research at three SSAP Symposia
- Visited LANL and LBNL to collaborate with research staff and present research results under SSAA funding
- Represented the NNSA on trips to LANL, LLNL, SNL, NNSS, LBNL, INL, PNNL, BNL, AFTAC, and the UK as an NNSA Graduate Fellow
- Traveled to the Boulby Underground Laboratory in England to coordinate a future NNSA research test bed



Stewardship Science Academic Alliances

The Multi-University Center of Excellence for Pulsed-Power-Driven High-Energy-Density Science

Cornell University ✦ PIs: Dr. David Hammer (dah5@cornell.edu) and Dr. Bruce Kusse (brk2@cornell.edu)

This Center combines the experimental, theoretical, and computational skills of six of the world's leading research universities to study the physics of pulsed-power-generated, high energy density (HED) plasmas. The experiments are designed to understand the dynamics of current-driven, HED, z-pinch implosions, many of which are done in collaborations of two or more Center partners. These experiments are supported by the extended magnetohydrodynamic (XMHD) computer simulations of PERSEUS (Cornell) and GORGON (Imperial College). Briefly discussed here are recent results from gas-puff, z-pinch experiments at Cornell, from the University of Michigan's Linear Transformer Driver (LTD) pulsed power machine, MAIZE, and from exploratory experiments testing the possibility of confining HED plasma produced by a wire array implosion in a magnetic mirror.

Research involving gas-puff z-pinches on Cornell's 1 MA COBRA pulsed-power machine uses a triple coaxial nozzle gas puff valve originally designed by colleagues at the Weizmann Institute of Science that enables the density profile to be adjusted to improve stability during implosion. Studies have focused on the implosion dynamics and stability of Ar, Ne, and Kr implosions at a peak current of 950 kA and a current rise time of 240 ns. Figure 1 shows the effects of gas species and neutral puff density during the gas-puff z-pinch implosions as described in the figure caption. The Kr results show dramatically different sheath structure and instability amplitudes that cannot be accounted for by the relative implosion accelerations. Effort is underway to fully characterize the plasma parameters in the imploding sheath for various initial conditions to better understand these differences and how they affect pinch dynamics.

The MAIZE pulsed power facility at the University of Michigan (a 0.5–1 MA LTD machine) completed an upgrade of its spark-gap switches in FY20 to simplify maintenance and to increase power and current delivery. Figure 2 shows a photo with all 40 switches firing. During FY20, MAIZE was used to study X-pinch X-ray sources, power flow experiments using three-dimensionally-printed electrode structures, and plasma jets produced by conical wire arrays for laboratory plasma astrophysics application. In addition, the first shots were taken with a new gas-puff z-pinch system that will be used with deuterium gas to enable studies of neutron production (including neutron imaging) from fusion reactions.

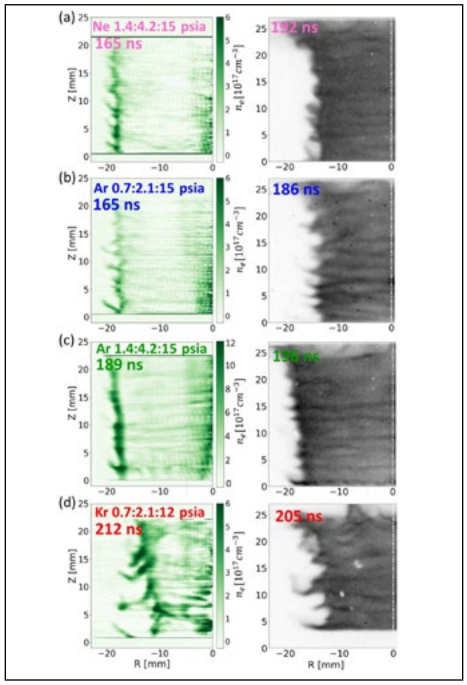


Figure 1. The effects of gas species and neutral puff density on the imploding plasma midway through a triple nozzle (outer annulus: inner annulus: central jet) gas-puff z-pinch implosions on the 1 MA COBRA generator. Left column: laser shearing interferometry measurements of plasma density. Right column, XUV self-emission images at nearly the same time. Panels a and b have approximately the same linear mass density, as do panels c and d, but show differences in magneto-Rayleigh-Taylor instability growth.

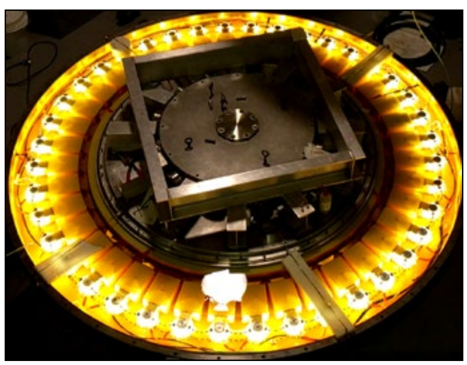


Figure 2. LTD Pulsed Power Machine MAIZE at the University of Michigan shown firing after being upgraded with 40 new switches.

A recently-initiated, exploratory study investigates magnetic-mirror confinement in a Magnitized Liner Inertial Fusion (MagLIF)-inspired concept in which the liner is simulated by an imploding, 4-wire cylindrical array. The mirror field is generated by spiraling wire feeds to the wire array at the anode and cathode ends. Extreme Ultra-Violet (XUV) pinhole camera images and interferometry monitor the effect of a mirror versus an open solenoidal field versus no field at all. XUV images are shown in Figure 3 together with diagrams of the three specified load configurations.

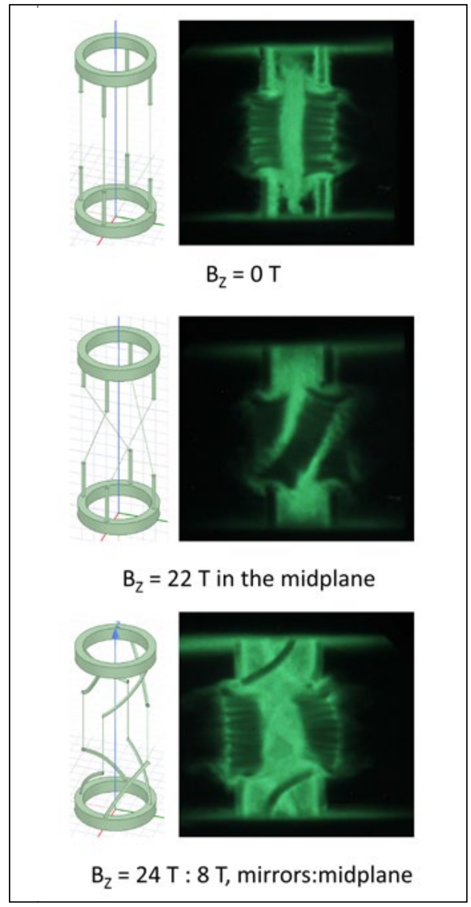


Figure 3. XUV images are shown together with the three specified load configurations when driven by 1 MA from COBRA.

The anode-cathode gap was 2.6 ± 0.1 cm, and the exposed wire section was 1.3 ± 0.1 cm long. Straight wires (Bz=0) produce typical ablation streams and instabilities. We used computer simulation to obtain estimates of the axial magnetic field produced by the loads at 1 MA. With straight current feed tubes and twisted wires in the middle generating 22 T, the field was likely too strong to allow an implosion. With the spiral current feed at the ends in the third configuration, the 3:1 mirror ratio with ~8 T in the middle appears to have allowed an implosion.

Center of Excellence for Advanced Nuclear Diagnostics and Platforms for ICF and HED Physics at Omega, NIF, and Z

Massachusetts Institute of Technology ✦ PI: Dr. Richard Petrasso (petrasso@psfc.mit.edu)

The first year of the Center of Excellence for Advanced Nuclear Diagnostics and Platforms for the Inertial Confinement Fusion (ICF) and High Energy Density (HED) Physics program resulted in a wide range of important research and student recruitment and training toward National Nuclear Security Administration (NNSA) objectives in high energy density physics (HEDP) and ICF by staff, postdoctoral fellows, PhD students, and undergraduate students at the Massachusetts Institute of Technology (MIT) and at its four partner institutions. The partners are the University of Iowa (UI) with Professor Scott Baalrud and PhD student David Bernstein; the University of Nevada Reno (UNR) with Professor Roberto Mancini and PhD students Dylan Cliche and Enac Gallardo-Diaz; the University of Rochester (UR) with Professor Riccardo Betti and postdoctoral fellow (now scientist) Dr. Jonathan Peebles; and the Virginia Polytechnic Institute and State University (Virginia Tech) with Professor Bhuvana Srinivasan and PhD student Megan McCracken. At MIT, there are eight graduate students (Patrick Adrian, Timothy Johnson, Neel Kabadi, Justin Kunimune, Brandon Lahmann, Ben Reichelt, and Graeme Sutcliffe) and one postdoctoral fellow (Arijit Bose). There have been six undergraduates at MIT in the Center, including Ryan Przybocki who recently graduated and moved to Stanford to study for a PhD in Physics; Ms. Hodaya Propp, a Cornell undergraduate doing summer intern work at MIT; Raymond Li, Bryan Sperry, Shaherul Haque, and Hugo Ramirez. One MIT PhD graduate and postdoctoral fellow, Hong Sio, left MIT last fall to work at Lawrence Livermore National Laboratory (LLNL), and one of the PhD students at UNR, Dylan Cliche, has graduated and now will be a postdoctoral fellow at LLNL. In total, Center participants have included three postdocs, 14 graduate students, and six undergraduates (Figure 1), all supervised by nine scientists and faculty at MIT and the partner institutions.

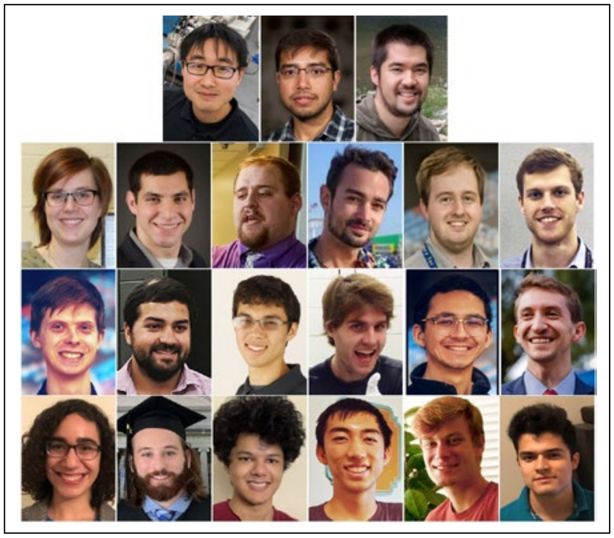


Figure 1. Center postdoctoral fellows (top row), PhD students (2nd and 3rd rows), and undergraduate students (bottom row).

Figure 2. Virginia Tech PhD student Megan McCracken and her thesis advisor, Professor Bhuvana Srinivasan (right), discuss their major simulation effort that includes multi-ion effects (be they for ICF implosions or for lab astro experiments). Nearly all other simulation codes, including HYDRA, LASNEX, FLASH, etc., are average-ion rather than multi-ion codes.

Most MIT students receive special laboratory training at the MIT HEDP accelerator facility. It was designed and built by students, run by students, and used by students to test and calibrate the many diagnostics they design and then operate at the National Ignition Facility (NIF) at LLNL, Omega and Omega EP at the UR Laboratory for Laser Energetics, and the Z machine at Sandia National Laboratories. Diagnostics currently under development by students or with student participation include cryoPXTD (for measuring the time histories of fusion products including charged particles and X-rays from cryogenic ICF implosions, as well as electron temperature evolution); the Knock-on-Deuteron Imager (KoDI) for observing the three-dimensional structure of ICF target shells with deuterium-tritium (DT) fuel; penumbral imaging of X-ray emission from ICF capsules; and MRSt, which will measure the DT-neutron spectrum as a function of time during ICF implosions at the NIF. Other diagnostics under development by students include a neutron spectrometer for the Z machine and a special three-particle backlighter for radiography of laser-driven ICF and laboratory astrophysics experiments with monoenergetic 3-MeV protons, 9.5-MeV deuterons, and 14.7-MeV protons (which a student is using to study electromagnetic fields in direct and indirect ICF and in laboratory astrophysics experiments). The students use the diagnostics to collect data they analyze for their own experiments and for supporting experiments performed by MIT collaborators. The students typically support approximately 100 NIF shots and 40 Omega shot days per year as well as attending weekly review meetings with NIF, Omega, and Z staff.

In addition to diagnostic development and experiments, the students do theoretical studies (e.g., particle transport in plasmas with and without magnetic fields). They run their own simulations of experiments with many existing codes (e.g., Hyades, Flash, RAGE, and iFP) and, in one case, develop their own simulation code for multi-ion-species shocks using the discontinuous Galerkin method (Figure 2).

Other important student and postdoctoral experiments have included studies of the effects of externally imposed magnetic fields on shock-driven ICF implosions; measurement of temperature disequilibrium of D and T ions in shock-driven implosions on Omega and the NIF; studies of ion-electron equilibration in plasmas; axial proton radiography of electric and magnetic fields inside laser-driven coils on Omega; studies of collisionless shocks and particle acceleration; and Omega X-ray spectroscopy of L-shell krypton emission for time-resolved measurements of electron density profiles.

Center for Excellence in Nuclear Training and University-based Research Pivots to Continue Experiment and Pipeline Development

Texas A&M University ✦ PI: Dr. Sherry Yennello (yennello@comp.tamu.edu); Author: Lauren McIntosh (centaur@comp.tamu.edu)

The past year has been full of unanticipated challenges and opportunities. The Center for Excellence in Nuclear Training and University-based Research (CENTAUR) has adjusted, pivoting to an online-only format for collaboration-wide meetings, Scientific Advisory Committee work, and a nuclear summer camp for early high school students. CENTAUR also continues research, making measurements within restrictions for social distancing and travel.

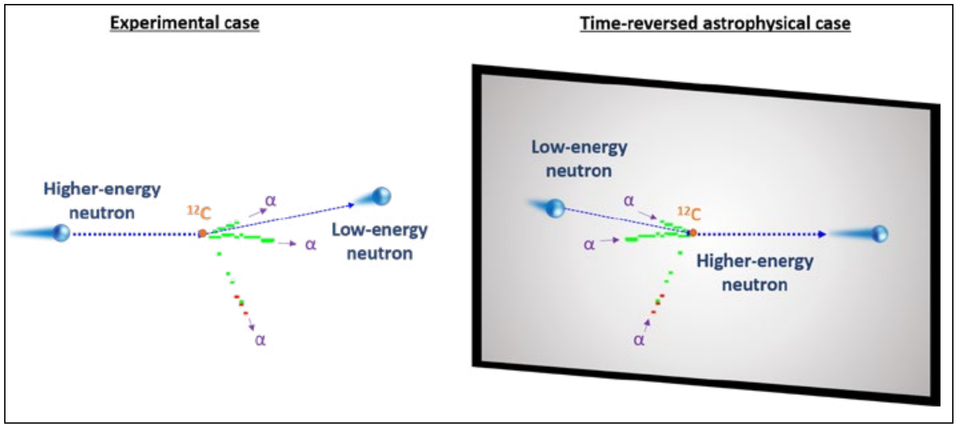


Figure 1. Left: Experimentally observed neutron-induced breakup of carbon-12 into three alpha-particles. Right: Time-reversed astrophysical case corresponding to formation of carbon-12 in the ground state via neutron upscattering.

One of the important measurements that was finished this year investigated the Hoyle state, a resonance in carbon-12. The triple-alpha process forming carbon is an important astrophysical reaction that depends upon the properties of the Hoyle state. These astrophysical reactions also may take place in a bath of neutrons, so the cross section for neutron-assisted de-excitation of ^{12}C in the excited Hoyle state to the ground state is of great interest at astrophysical energies.

Direct measurement of this reaction (or its reverse) historically has been impossible due to high neutron background at neutron beam facilities. TexAT, an active target detector developed by the group of Professor Grigory Rogachev (Texas A&M University (TAMU)), offered the opportunity to detect the tracks of all three alpha particles which make a characteristic trident-shaped track in the detector (Figure 1). The experiment, proposed by Professor Lee Sobotka (Washington University in St Louis), used a highly-collimated, mono-energetic neutron beam produced using the d(d,n) reaction at the Edwards Accelerator Laboratory (EAL) at Ohio University impinging into the active target area of TexAT to make the cross-section measurement over a wide energy range of neutrons by detecting the resultant alpha particles from the decay of the Hoyle state.

The experiment was well underway in March when the global COVID-19 pandemic was declared. Anticipating local lockdowns under guidance from collaborators at EAL, CENTAUR participants went home, leaving TexAT in-line ready to take neutrons as soon as the accelerator was able to run. Once travel guidelines were in place, two postdoctoral researchers from TAMU, following COVID-19 guidelines, returned to finish gathering data culminating in >300 hours of measurements. A recent Scientific American article highlighted the significance of this CENTAUR experiment.

Some challenges were overcome, not by traveling within new restrictions but by bringing experiments to students' homes. The Nuclear Medicine and Science Camp spearheaded by Professor Paul Cottle (Florida State University (FSU)), went to a fully-online format this year. Nineteen high school students were able to participate in the camp in the summer of 2020, which is on the order of the number who have participated in previous years. The camp was taught by Professor Cottle and two local high school teachers in the Florida panhandle.

The instructors refused to skip the most important part of this learning experience—the experiments. They packed up a box for each student which contained a Ludlum survey meter and Alpha-Beta-Gamma detector, a PASCO gamma source, gamma absorbers, 'No Salt' sample, and other supplies. The students' families picked up the box at the beginning of the week and delivered the box back at the end of the week (Figure 2).

Figure 2. Parents and campers returned their equipment boxes from home on the last day of camp at FSU's Panama City (PC) campus. From left, FSU-PC Science, Technology, Engineering, and Mathematics Institute Director, Ginger Littleton, teacher Ms. Denise Newsome, camper Joe Hovis (holding his camp certificate), and teacher Ms. Paige Johnston.

In addition to at-home experiments with gamma absorption, the campers virtually toured the Los Alamos Neutron Science Center (LANSCE) at Los Alamos National Laboratory and the Gulf Coast Regional Medical Facility's nuclear medicine facility. They attended a lecture on astrophysics from another FSU faculty member. The campers also were able to control parameters of gamma spectroscopy software from their homes over the Internet. The ability to run such a nuclear summer camp remotely opens up new possibilities for expansion in the future. This time of social distancing has required CENTAUR, with members in six different states, to collaborate in new ways.

Center for Research Excellence on Dynamically Deformed Solids

Texas A&M University ✦ PI: Dr. M.J. Demkowicz (demkowicz@tamu.edu)

With the advent of additive manufacturing, there is a growing need to understand and control materials with complex, multi-phase microstructures. The aggregate behavior of such materials depends on the properties, shapes, and arrangement of their many constituents as well as on the interfaces between the constituents. The goal of the Center for Research Excellence on Dynamically Deformed Solids (CREDDS) is to build up the fundamental understanding needed to predict the performance of advanced, multiphase materials when deformed at very high rates of strain in excess of 10^4/s.

A collaboration between four research universities (Texas A&M University, University of Michigan, University of Connecticut, and University of California in Santa Barbara (UC-Santa Barbara)), CREDDS supports 17 PhD students to address these materials science challenges in collaboration with the National Nuclear Security Administration (NNSA) laboratories. In 2020, five of these students had semester-long internships at Los Alamos National Laboratory (LANL), Lawrence Livermore National Laboratory (LLNL), or Sandia National Laboratories (SNL). Working with technical staff member John Mitchell from SNL, Texas A&M University (TAMU) PhD student Edwin Chiu (Figure 1) learned the hydrocode Alegra and used it to model high velocity impact and spall fracture. The objectives were to implement a polycrystalline microstructure and observe its influence on face velocity as well as to improve predictions of microstructure-dependent material properties. During his stay, Edwin extended his work to the modeling of hole closure via high velocity impact.

Ethan Sprague, a PhD student from the University of Michigan, worked at the Advanced Manufacturing Facility at LLNL on pyrometry calibration and collection under the guidance of staff member Ibo Matthews. Ethan used the data he collected to identify strut and overhang defects in 316L stainless steel parts built by Selective Laser Melting (SLM). In the summer of 2020, Ethan continued to collaborate with LLNL remotely, working with staff member Gabe Guss on developing tools for three-dimensional viewing of pyrometry data collected during the SLM process. To that end, Ethan implemented a computer model to predict heat buildup and melt pool depth as a laser scan rasters into a corner, along an edge, or at any other location where heat is liable to build up and affect SLM part quality.

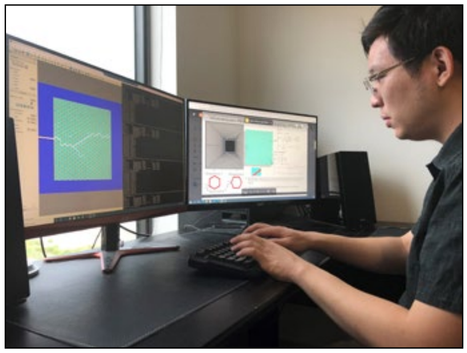


Figure 1. TAMU PhD student Edwin Chiu.

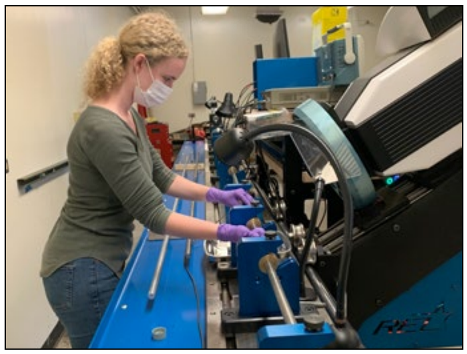


Figure 2. UC-Santa Barbara PhD student Lauren Poole.

One advantage of the close relationship between the Center and NNSA laboratories is that it creates opportunities for CREDDS members to transition to full-time employment at the laboratories. Last year, two CREDDS alumni joined LANL. Dr. Zachary Levin, a former CREDDS postdoctoral fellow at Texas A&M, now is a technical staff member in the MST-16 group at LANL. He is an expert in material processing by severe plastic deformation. Dr. Benjamin Derby, former CREDDS PhD student at the University of Michigan, now is a postdoctoral researcher at the Center for Integrated Nanotechnologies (CINT). His expertise lies in physical vapor deposition and electron microscopy.

Experimental researchers faced unprecedented challenges in 2020 due to facility closures. Several CREDDS members used these circumstances as an opportunity to augment existing experimental efforts with new modeling insights. For example, Texas A&M PhD students Liya Semenchenko and Emmeline Sheu gained new skills in finite element modeling using the ABAQUS and MOOSE software packages. As facilities began to re-open, CREDDS students adopted new procedures that enabled them to progress in their research while maintaining a safe working environment. For example, UC-Santa Barbara PhD student Lauren Poole (Figure 2) resumed her work using the split Hopkinson pressure bar for high strain rate compression testing of multiphase materials.

Figure 3. Pictured are 9 of the 13 undergraduate researchers who participated in internships sponsored by CREDDS during summer 2020.

In addition to finding new avenues for continued productivity among its own members, CREDDS undertook two major outreach activities in response to the COVID-19 crisis. The first was to develop and host the 2020 online summer school on dynamic deformation of solids (SSDDS). The school consisted of 13 weekly lectures and review sessions delivered via Webex by faculty at U.S. academic institutions and technical staff at the NNSA laboratories. Over 160 individuals registered for the summer school, representing a wide range of universities, several national laboratories and user facilities, and industry. SSDDS lectures and review sessions were recorded and made available on a dedicated YouTube channel (https://www.youtube.com/channel/UCu3F29xeWUm23zcvGdtEctw), providing a permanent resource for the research community working on dynamic deformation of solids. The second activity was to engage 13 undergraduate researchers from around the United States in online summer research internships: two at the University of Michigan and 11 at Texas A&M, 9 of whom are shown in Figure 3. These undergraduate research internships expose students to the materials challenges addressed by CREDDS and build their interest in technical careers at the NNSA laboratories.

Center for Matter Under Extreme Conditions

University of California, San Diego ✦ PI: Dr. Farhat Beg (fbeg@ucsd.edu)

The Center of Excellence for Matter under Extreme Conditions (CMEC) is a unique collaboration between scientists in High Energy Density Physics (HEDP) from academia, national laboratories, and industry. This past year, 14 CMEC graduate students conducted research in cutting-edge HEDP topics in collaboration with the national laboratories. Two examples are showcased in this article.

Pertinent to the Center's progress on matter under extreme pressure and temperature conditions, dynamic natural processes are being modeled that require both integration of material properties and the material response to external forces (e.g., acceleration of energetic particles). This work is led by postdoctoral fellow Felipe González-Cataldo and his advisor Burkhard Militzer at the University of California (UC) Berkeley. Figure 1 shows predictions from first-principles computer simulation for the shock Hugoniot curve of elemental magnesium and a comparison with the corresponding curves of oxygen and MgO.[1] The different maxima in compression are caused by the excitations of the different electronic shells that triggered thermal ionization. The maximum at lower pressures of 10^4 GPa is caused by the ionization of L-shell electrons, whereas the maximum at $3\text{x}10^5$ GPa is introduced by ionization of the K-shell. Radiation effects are highlighted by the green-shaded area, and correction due to relativistic effects are indicated in grey. All curves were obtained from a recently-published equations of state table that was derived with path integral Monte Carlo and density functional molecular dynamics simulations. A multi-shock analysis predicted how close one can get to an isentrope with multi-shock experiments. The electronic density of states were analyzed to illustrate how the energy bands merge and how electrons are promoted to the conduction band as a function of temperature and pressure.[2]

State-of-the-art, high-power lasers, like the National Ignition Facility (NIF), facilitate unraveling of the material's response in the extreme regime using shock and isentropic compression. In order to better understand and constrain models for high-strain-rate processes, material properties at these extreme conditions need to be properly determined. The research conducted by graduate student Gaia Righi and her advisor Marc Meyers at UC San Diego is relevant to planetary science since they are: (a) establishing the strength of iron in the Earth's core and (b) unraveling the details of the deformation of olivine and forsterite, major components of the Earth's mantle. In these experiments, a hohlraum geometry was used to generate high-power X-rays to drive a sample. The NIF enables us to drive iron to 350 GPa and 4,000 K, and radiography makes it possible to measure Rayleigh-Taylor growth factors, which then are compared to strength models to infer strength of the material. The preliminary results show that iron is stronger than the models predict and that there is little to no difference in growth factor and, consequently, strength between fine-grained and monocrystalline iron. It is thought that the formation of a nanostructure during shock (Figure 2) plays a role in this unusually high strength, but more development and inquiry into the fundamental deformation mechanisms are needed. This study will continue in future campaigns.

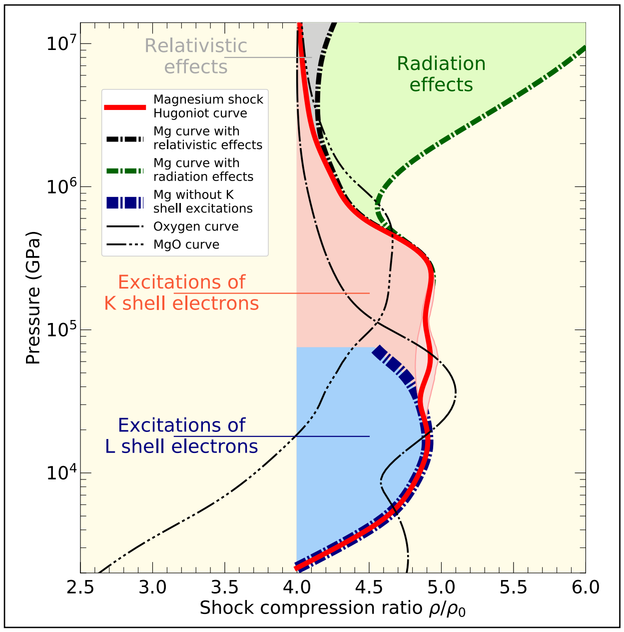


Figure 1. Shock Hugoniot simulation for magnesium is compared with results for oxygen and magnesium oxide. Densities are divided by the initial density of ρ_0= 1.737 gcm^{-3}. The broad temperature interval from 250,000 to 1.6×10^7 K, where the Mg curve exceeds a compression ratio 4, can be attributed to ionization of the K and L shell electrons. Relativistic and radiation effects only become important at the highest pressures.

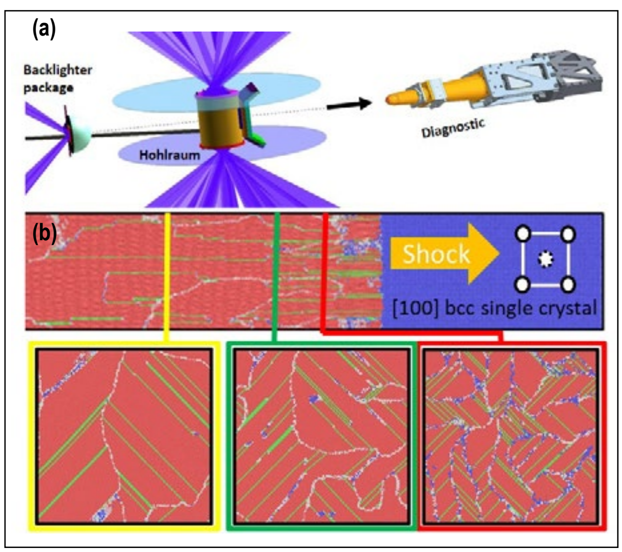


Figure 2. (a) Experimental setup at the NIF. Hohlraum is illuminated by 192 beams, and backlighter illuminates target for side-on radiography. (b) Molecular dynamics simulation of iron subjected to 55 GPa shock. The top image shows shock wave passing through single crystal bcc iron. The bottom image shows evolution of nanostructure as shock passes through. Colors represent different phases: blue = BCC, green = FCC, red = HCP, white = unidentified.

To expand CMEC's educational reach to the greater United States, the Center teamed up with the Center for High Energy Density Physics at Lawrence Livermore National Laboratory to offer a four-credit course on "Diagnostics for High Energy Density (HED) Plasmas." The course was offered through Webex and was attended by more than 250 graduate students, postdoctoral fellows, and scientists.

References

[1]F. Gonzalez-Cataldo, F. Soubiran, and B. Militzer, "Equation of State of Hot, Dense Magnesium Derived with First-Principles Computer Simulations," Phys. Plasmas 27, 092706 (2020). DOI: 10.1063/5.0017555.

[2]F. Gonzalez-Cataldo, F. Soubiran, H. Peterson, and B. Militzer, "Path Integral Monte Carlo and Density Functional Molecular Dynamics Simulations of Warm, Dense MgSiO3," Phys. Rev. B 101, 024107 (2020).

CDAC Begins a New Phase as the Chicago/DOE Alliance Center

University of Illinois at Chicago ✦ PIs: Dr. Russell J. Hemley (rhemley@uic.edu) and Dr. Stephen A.Gramsch (sgramsch@uic.edu)

The Chicago/DOE Alliance Center (CDAC), headquartered at the University of Illinois at Chicago, builds a coalition of partners focused on the research of materials at extreme conditions. The Chicago location places the Center in close proximity to the other academic partners, and to the facilities of the High Pressure Collaborative Access Team (HPCAT), the dedicated extreme conditions beamline at the Advanced Photon Source (APS) at Argonne National Laboratory. Interactions with other SSAA Centers as well as with other NNSA-supported activities at APS are enabled by the Chicago location.

Student training remains the focus of CDAC and, for the first time, the Center will host its own graduate students from many disciplines in both science and engineering, including both experiment and theory. Situated just a mile from downtown Chicago, UIC is recognized by the U.S. Department of Education as a Minority Serving Institution and contains the administrative resources and expertise to foster effective outreach to students from groups that are underrepresented in scientific and technical disciplines. It is an important goal of CDAC to facilitate this aspect of workforce development in support of the National Nuclear Security Administration.

CDAC staff at UIC consists of Director Russell Hemley, Deputy Director Stephen Gramsch, and Research Professors Muhtar Ahart, Ravhi Kumar and Zhenxian Liu, the onsite coordinator of the Frontier Infrared Spectroscopy (FIS) facility at the National Synchrotron Light Source-II at Brookhaven National Laboratory. The Academic Partner group counts among its members Steven Jacobsen (Northwestern University), Eva Zurek (University at Buffalo), Lowell Miyagi (University of Utah), Susannah Dorfman (Michigan State University), Maik Lang (University of Tennessee), and Elif Ertekin (University of Illinois at Urbana-Champaign).

The CDAC scientific program consists of seven key Center thrusts: Elasticity and Equations of State, Plasticity, Strength and Deformation, Complex Materials, Extreme Chemistry, Defects and Ion Irradiation, Phase Transition Dynamics, and Superconductivity. The CDAC laboratory at UIC will host comprehensive sample preparation and optical spectroscopy facilities to complement the capabilities of other Center laboratories in the support of Center scientific and training programs. In addition, the UIC laboratories are available for inter-Center collaborations and training for personnel seeking to engage in extreme conditions research at HPCAT.

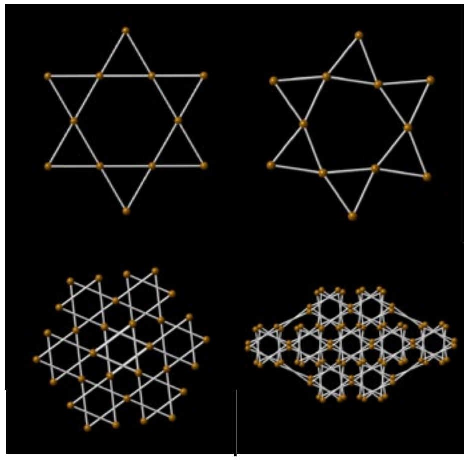


Figure 1.Kagomé net of Fe^{3+} centers in jarosite. Top: Structural unit of the net at (left) ambient pressure and (right) 80 GPa. Bottom: Layers of extended nets at (left) ambient pressure and (right) 80 GPa.

The availability of synchrotron techniques has enabled numerous advances in the study of materials at extreme conditions, and the physics of materials with correlated electrons and their behavior at high pressure has been an ongoing area of emphasis. Recently, the Jacobsen group at Northwestern University used multiple synchrotron methods in a study of the frustrated antiferromagnetic material jarosite, $KFe_3(OH)_6(SO_4)_2$, which combined results from X-ray diffraction and X-ray emission spectroscopy at HPCAT, synchrotron Mössbauer spectroscopy at APS Sector 3, and synchrotron infrared spectroscopy at FIS.[1] At approximately 45 GPa, the Kagomé net of Fe^{3+} centers undergoes a collapse of magnetic order accommodated by the formation of an unusual twisted net in which the triangular geometry of the equilateral triangles of Fe^{3+} ions is preserved (Figure 1).

In an outgrowth of longstanding CDAC research on the growth of large, single crystal diamond by chemical vapor deposition (CVD), a collaboration between Penn State University and CDAC has resulted in the first silicon optical fibers encapsulated by diamond grown by CVD methods (Figure 2). These fibers, which have a homogeneous diamond morphology over their entire length, have been shown to guide infrared light and may provide significant enhancements in remote sensing and structural monitoring in extreme environments or when probing for chemical signatures at mid-infrared wavelengths.[2]

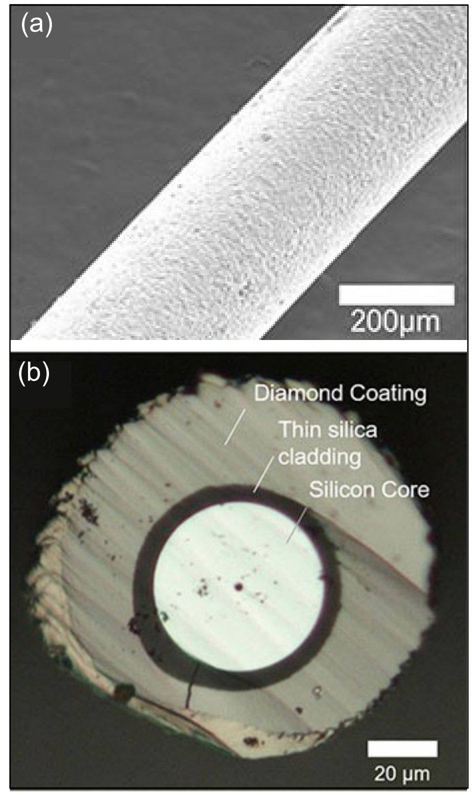


Figure 2. (a) Scanning electron microscope image of diamond encapsulated silicon fiber showing homogeneous morphology. (b) Cross section of a 50 micron silicon fiber after polishing in an ion mill. The fiber is clad in a thin layer of silica and coated in diamond.

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The Center for Laboratory Astrophysics

University of Michigan ✦ PI: Dr. Carolyn Kuranz (ckuranz@umich.edu)

The Center for Laboratory Astrophysics (CLA) studies high-energy-density (HED) science relevant to astrophysical phenomena in three main areas: Radiation Hydrodynamics, Complex Hydrodynamics and Hydrodynamic Instabilities, and Magnetized Flowing Plasmas. Whereas the main work of CLA is experimental, with experiments performed at a variety of HED facilities, they also perform radiation hydrodynamic simulations using the CRASH code, a multigroup, flux-limited diffusion, radiation hydrodynamics code. According to Dr. Carolyn Kuranz, the Center Director and an Associate Professor at the University of Michigan, "CLA researches fundamental HED physics relevant to astrophysics and the NNSA mission. We pride ourselves in the holistic education of junior scientists in HED science." The Center currently has nine graduate students and a postdoctoral fellow mentored by Professor Kuranz and Emeritus Professor R. Paul Drake. Figure 1 shows Director Kuranz and former CLA graduate student Dr. Laura Elgin at the Omega Laser Facility discussing an experiment. CLA students often work closely with scientists and engineers at NNSA laboratories and NNSA facilities as part of their doctoral work.

Figure 1. CLA Director Carolyn Kuranz and former CLA graduate student Dr. Laura Elgin, currently a staff member at Sandia National Laboratories, discussing a hydrodynamic instability experiment at the Omega Laser Facility in Rochester, NY. Image credit: Eugene Kowaluk, LLE

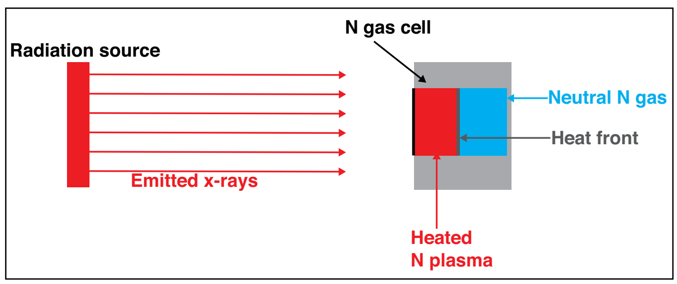

Figure 2. Schematic of a photoionization front experiment where an x-ray source is incident on a nitrogen gas cell. Image Credit: Heath LeFevre, University of Michigan

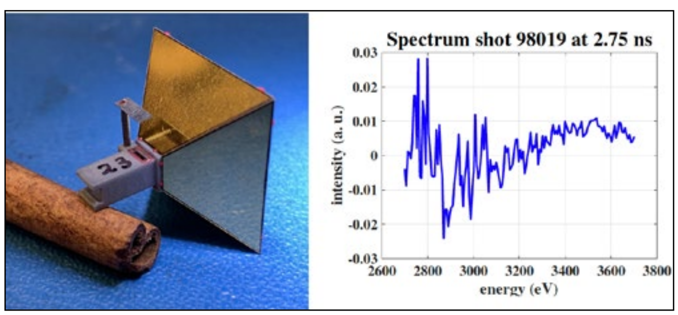

Figure 3. A target for the Omega Laser Facility (left) and a preliminary absorption spectrum (right). Image credit: Sallee Klein and Heath LeFevre, University of Michigan

Specifically, for their radiation hydrodynamics work, CLA researchers study how radiation interacts with matter. They have extensively studied the evolution of radiative shocks at the Omega Laser Facility and the National Ignition Facility. More recently they have begun developing a platform to study photoionization (PI) fronts, which are a type of heat wave where radiation propagates through a cold material and causes ionization and heating dominated by photon interactions with atoms. It is believed that these fronts were ubiquitous during the early Universe as it emerged from the so called 'Cosmic Dark Ages'. This was, in part, due to stellar radiation from the first stars ionizing and heating the surrounding gas. PI fronts are also important in the transition between pre-planetary to planetary nebula during the late-stage evolution of intermediate mass stars and have important effects on the gas surrounding stars, from destroying giant molecular clouds, affecting future star formation, and even limiting the final stellar mass of a high mass protostellar object. The conditions for a PI front are sensitive to radiation transport and the atomic physics in complex materials. CLA researchers are working to determine the conditions to create a PI front and to observe its evolution in the laboratory.

CLA is using both the Z machine at Sandia National Laboratories and the Omega Laser Facility at the University of Rochester for complementary experiments to create and characterize a PI front. In both experiments, an X-ray radiation source is generated either with a dynamic hohlraum on Z or by a laser-irradiated gold foil on Omega. The radiation then is incident on a gas cell containing a nitrogen gas at 5-10 atm. A schematic of the fundamental experiment is shown in Figure 2. They will use various spectroscopy techniques to diagnose the experiment, ideally observing the propagation of the moving interface between the hot, ionized gas and the cold, neutral gas. Figure 3 (left) shows a target for the Omega Laser Facility resting on a cinnamon stick for scale, and (right) preliminary data from a PI front experiment. The experiments initially were performed and designed by University of Michigan graduate student Heath LeFevre with fellow graduate students Michael Springstead and Kwyntero Kelso leading the upcoming experiments at Z and Omega, respectively. This work includes close collaborations with scientists and technicians at the Omega Laser Facility in Rochester, New York and Z at Sandia National Laboratories.

CLA will continue these campaigns on Z and the Omega Laser Facility. Additionally, they are exploring hydrodynamic instability experiments on the National Ignition Facility and the Omega Laser Facility, investigating the Kelvin-Helmholtz instability, Rayleigh-Taylor instability, and the onset of turbulence in the HED regime. CLA students also are using the 1-MA MAIZE pulsed power facility at the University of Michigan, led by Professor Ryan McBride, to study magnetized plasma flows.

Actinide Center of Excellence: New Actinide Materials and Radiation Durability

University of Notre Dame ✦ PI: Dr. Peter C. Burns (pburns@nd.edu)

The mission of the Actinide Center of Excellence (ACE) is to conduct research in actinide chemistry and materials with an integration of experimental and computational approaches and an emphasis on research questions and priorities that are important for the security of the Nation via stockpile stewardship with workforce development as a motivating goal. ACE is working to develop a fundamental scientific understanding of the actinides. All are radioactive, and those heavier than uranium are synthetic. Actinides fuel nuclear weapons and reactors that generate 20% of our electricity. They propel naval vessels and are used to produce medical isotopes. They also are environmental contaminants at weapons-related sites. Understanding actinide chemistry helps to predict the aging of actinide-based weapon components and to control these elements in all of their forms. Researchers in ACE discover new actinide materials and study stabilities, transformations, and properties of actinide materials under changing temperature, pressure, and radiation conditions.

Metal organic frameworks (MOFs) combine metal-oxide nodes with organic linkers to produce highly-porous materials with applications including chemical separation and purification, catalysis, sensing, and gas storage. Students in ACE synthetically prepared several fascinating actinide-based MOFs and studied their properties. Amongst these is the first MOF containing plutonium[1] (Figure 1) and the first to contain neptunium in its pentavalent oxidation state.[2] The plutonium MOF extends a family of tetravalent-metal MOFs deeper into the actinide series,[1] and the neptunium MOF is based on a new cluster consisting of eighteen neptunium cations and oxygen.[2]

Upon removal from a reactor, an actinide fuel is intensely radioactive largely due to fission products. Materials used in separation and purification of components of irradiated fuel and fabrication of waste forms receive high radiation doses that can dramatically change material properties. ACE students use Co-60 gamma sources to irradiate actinide materials in bulk and a helium ion beam from an accelerator to simulate the effect of alpha particles (an alpha particle is identical to a helium nucleus). ACE researchers then use X-ray scattering and spectroscopic methods to determine the extent of damage in an actinide material arising from specific quantities and types of radiation.

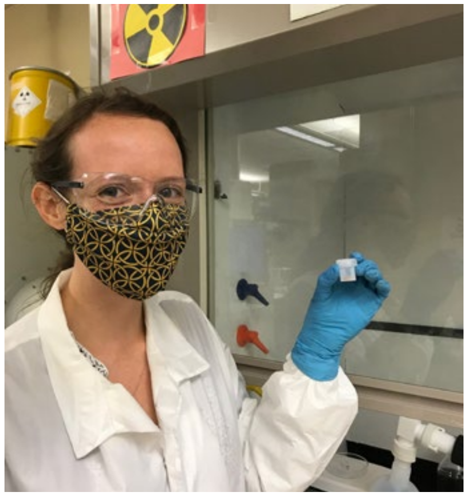

Figure 1. ACE PhD student Ashley Hastings holding a Teflon vessel containing the world's first plutonium-based metal organic framework (MOF) compound.[1]

Radiation levels encountered in the nuclear fuel cycle can render materials ineffective for their intended purpose in separation and purification of fuel components as well as waste storage. MOFs have valuable properties, but will they survive such challenging environments? It is essential to understand their response to extreme radiation doses and to design MOF compositions and structures that are highly durable.

ACE students designed and synthesized a new thorium-binaphthol MOF containing thorium oxide nodes (Figure 2) and set out to destroy it by irradiation. As a point of reference, a radiation dose of eight Gray (Gy) is lethal to humans. The new MOF showed no sign of damage after four MGy (four million Gy) of gamma irradiation and holds the record as the most radiation-resistant MOF. During the first study of the stability of a MOF during helium ion beam irradiation to simulate alpha particles, ACE students found that their new MOF began showing signs of damage at 15 MGy of irradiation and that it was destroyed by 25 MGy of irradiation. This tremendous resistance of radiation damage demonstrates that MOFs can be used in high radiation environments, such as in chemical separations and waste applications in nuclear fuel cycles.

ACE Principal Investigator Professor Burns noted "our Center structure and funding is providing ACE students with a myriad of opportunities to learn in a collaborative research environment, and I am very impressed by their accomplishments in the area of actinide-based MOFs."

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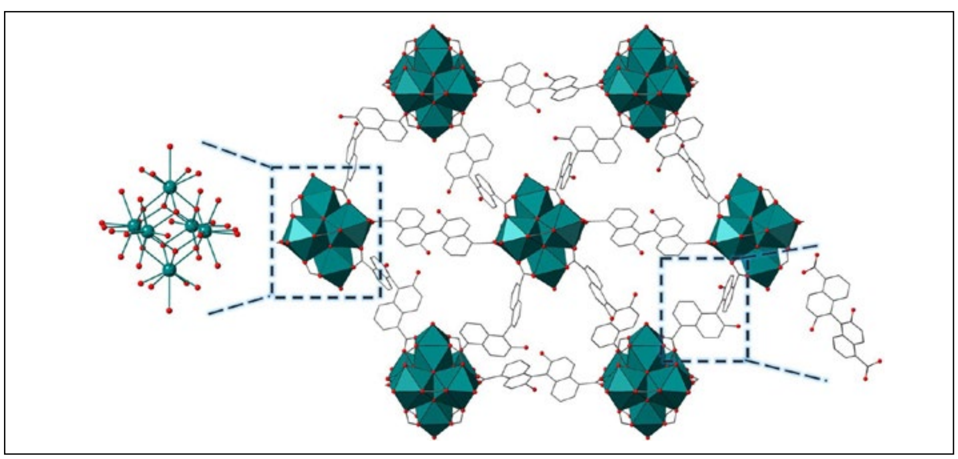

Figure 2. The structure of the new thorium-based MOF that holds the record of being the most radiation resistant.[3] The structure consists of thorium oxide nodes (shown on left) and binaphthol linkers (right). Th, O and C are shown in blue, red, and grey, respectively.

The Wootton Center for Astrophysical Plasma Properties

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The purpose of the Wootton Center for Astrophysical Plasma Properties (WCAPP) is to explore matter under a wide variety of cosmic conditions in the laboratory, transforming astrophysics into an experimental science. WCAPP enables graduate students and postdoctoral researchers to work in a national laboratory, scientific culture and to gain expertise in theoretical and experimental atomic physics, spectroscopy, and platform development, which prepares them to lead in these areas. Fundamental science experiments are conducted at the Z pulsed power facility (Z) at Sandia National Laboratories (SNL) with other experiments proposed for the National Ignition Facility (NIF). At present, WCAPP carries out four independent, astrophysically-motivated experiments simultaneously on each shot. There have been two shot series in the past year. Each has led to significant progress on all four experiments.

Over the past year, the white dwarf team has made experimental and theoretical advances in our understanding of the fundamental properties of white dwarf stars. Marc Schaueble (former graduate student, now SNL staff member) led the publication of results for the hydrogen experiments, highlighting an inconsistency in the measured electron density when using two different hydrogen lines.[1] Patty Cho (Figure 1) has been incorporating a new generation of hydrogen line calculations into model white dwarf atmospheres using models developed by Thomas Gomez (former graduate student, now an SNL postdoctoral fellow). She is transitioning to work with Guillaume Loisel on his Accretion-Powered Matter and Radiation experiment. In two shot series, postdoctoral fellow Bart Dunlap has led experiments on carbon plasmas at conditions relevant to white dwarfs with carbon-dominated atmospheres. These stars likely are the result of mergers of two white dwarfs and are important for understanding type Ia supernovae.

The Accretion-Powered Matter experiment explores the conditions in disks around compact objects such as black holes or neutron stars where copious amounts of X-rays are generated. These objects emit spectra that contain information about the accretion process and the nature of the accretor. The Z facility recreates the

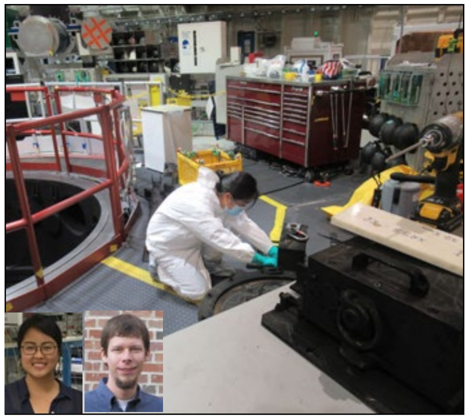

Figure 1. Senior graduate student and LRGF 2020 award winner Patty Cho (above and lower left) at work near the center section of the Z machine. WCAPP postdoctoral fellow and team leader of the white dwarf experiment, Bart Dunlap (lower right).

relevant state of X-ray photoionization of the radiation-dominated disk environment and its spectral emission.[2] One feature of the emission is the radiative recombination continuum (RRC) which is used as an important diagnostic of disk temperature. Guillaume Loisel and his team have used Z to make the first-ever laboratory measurements of RRC (Figure 2) made at astrophysical conditions. These will serve as benchmarks for this important accretion disk temperature diagnostic. Roberto Mancini and students Daniel Mayes and Kyle Swanson study the ionization, X-ray heating, and electron temperature of photoionized plasmas relevant to astrophysics. They employed a novel method to measure electron temperature independently of atomic kinetics modeling and have demonstrated the dramatic impact of photoexcitation driven by a broadband X-ray flux on excited level populations, radiation cooling, and the energy balance of photoionized plasmas. Predictions of astrophysical codes significantly overestimated the measured temperature.[3] Their Z experiment has enabled the first observation of the charged state distribution evolution as a function of the ionization parameter. These results are setting unprecedented tight constraints on modeling codes. The latter constituted the central theme of the PhD dissertation of Daniel Mayes (Figure 3) who graduated in December 2020.

The stellar opacity experiment has continued work to build on the landmark measurement of Bailey et al.[4] of iron opacity at the conditions of the base of the solar convection zone. Whereas the

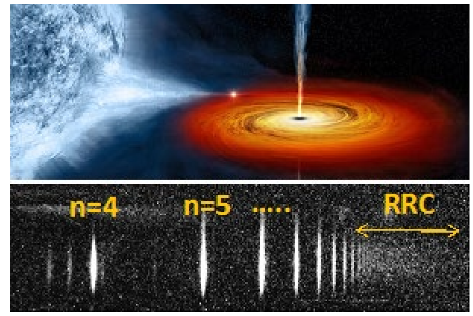

Figure 2.The first radiative recombination continuum measurements (RRC) have been made as part of the Accretion-Powered Matter and Radiation experiment.

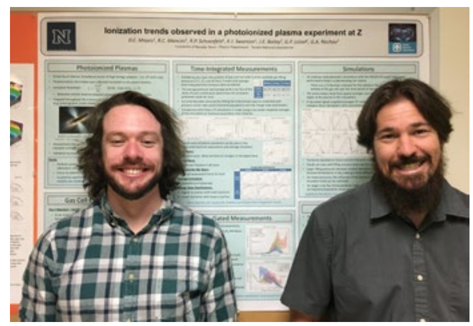

Figure 3. Students Kyle Swanson (left) and Daniel Mayes (right) showing their poster on observation of ionization trends in the neon gas cell experiment at Z.

recent reanalysis slightly reduced the discrepancy between the measured and theoretically predicted opacity of iron, significant disagreement still exists to date. Additional iron opacity measurements were obtained to consolidate the accuracy of the iron result. The Ultrafast X-ray Imager spectrometer on Z allows the experimenters to observe how the opacity-sample conditions evolve over time which will improve the understanding of the experiments, suggest experimental refinements, and allow them to quantify the impact of temporal gradients on the published results. They performed the first oxygen-opacity experiment to test the accuracy of opacity models for this highest opacity contributor at the base of the solar convection zone.

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Statistical Nuclear Properties

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The statistical properties of nuclei and cross sections of (α,n) reactions are essential data for a variety of nuclear applications and problems in nuclear astrophysics. Since May 2019, Stewardship Science Academic Alliances (SSAA) has supported a dedicated research effort at the Edwards Accelerator Laboratory at Ohio University that is aimed at obtaining such data and advancing the associated experimental techniques. This work has been led by faculty members Zach Meisel and Alexander Voinov along with graduate students Kristyn Brandenburg and Michael Hartos (now at The University of Utah).

Most modeling problems in nuclear applications, including stockpile stewardship and nuclear astrophysics, involve computing reactions and decays involving a large number of nuclides. Measuring the structure properties and reaction probabilities for all nuclides and reaction scenarios is not practicable in general. As such, theoretical models generally are employed. Chief among these for medium and heavy nuclides is the Hauser-Feshbach statistical formalism. Hauser-Feshbach calculations require estimates for statistical nuclear properties such as the average density of nuclear states at a given nuclear excitation energy and quantities related to the probability of emitting or absorbing a photon, neutron, or charged particle, known as transmission coefficients. Mapping the evolution of these properties across the nuclear landscape is necessary to ensure accurate calculations.

A major focus of this program has been the determination of statistical nuclear properties using particle evaporation spectra from nuclear reactions. In these measurements, a light projectile nucleus fuses with a heavier target resulting in a compound nucleus that subsequently boils-off light particles. Statistical nuclear properties can be gleaned from the particle energy and angular distributions as well as the relative yield of different particle types. For nucleons and alpha-particles, the transmission coefficients are related directly to optical potentials in analogy to light scattering on an opaque disk.

One quantity of interest is the nuclear level density, a count of the number of nuclear excited states within a given excitation energy window, which is expected to increase roughly exponentially with increasing excitation energy. Theoretical predictions often vary by more than a factor of a few, with a correspondingly large impact on associated nuclear reaction rates. This research involved measuring protons emitted following the bombardment of zinc targets with a lithium beam, finding[1] that the nuclear level density of ^{74}Ge and ^{76}Ge are significantly lower than all commonly used theoretical predictions. Similar experiments included a simultaneous measurement of protons, α-particles, and neutrons emitted from boron bombarding a calcium target. Protons and αs were distinguished with a spectrometer measuring the particle's time-of-flight and energy (Figure 1). Neutrons also used time-of-flight. Preliminary results indicate a reduction in the neutron emission probability relative to expectations.

“Each of the experimental efforts in this research have provided valuable training opportunities for SSAA students. Along with expertise in statistical nuclear physics, students have gained experience in bread-and-butter particle detection techniques that feature prominently in National Nuclear Security Administration programmatic work.”

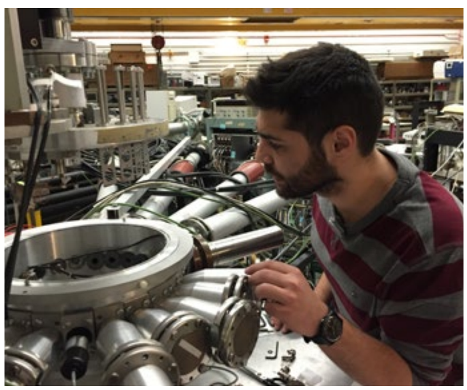

Figure 1. Charged-particle time-of-flight chamber used for charged-particle evaporation spectrum measurements.

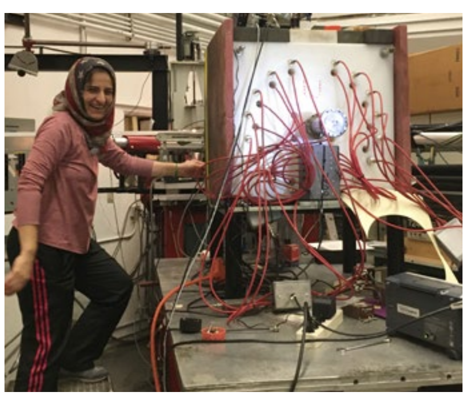

Figure 2.The HeBGB neutron detector for (α,n) measurements.

Another focus of this program has been the direct measurement of α-capture neutron-emission (α,n) reaction cross sections. These cross sections not only help constrain the highly uncertain optical potential for α-particles but often are of direct interest. In particular, (α,n) reactions feature prominently in actinide rich environments and several explosive astrophysical scenarios. In the past year, the ^{3}He BF_3 Giant Barrel (HeBGB) detector (Figure 2), dedicated for (α,n) cross section measurements, has been completed. First measurements focused on ^{27}Al(α,n) in an energy regime where existing data is sparse. This reaction is of direct interest for actinide-rich conditions as well as the synthesis of the supernova diagnostic ^{44}Ti.

Each of the experimental efforts in this research have provided valuable training opportunities for SSAA students. Along with expertise in statistical nuclear physics, students have gained experience in bread-and-butter particle detection techniques that feature prominently in National Nuclear Security Administration programmatic work.

Reference

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Maximizing Reliability and Information Content of Ramp Compression Experiments with *In Situ* X-ray Characterization

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The expansion and accessibility of X-ray user facilities paired with dynamic loading creates exciting prospects for asking scientific questions about high-pressure behavior across a wide range of strain rates and pressure and temperature states. The goal of this academic program is to investigate the behavior of materials under ramp compression using *in situ* X-ray scattering techniques at the Dynamic Compression Sector (DCS), Advanced Photon Source. This new program represents a first collaboration of PIs Todd Hufnagel and June Wicks from Johns Hopkins University (JHU), bringing together complementary research programs using X-ray scattering techniques and high pressure experiments at user facilities around the country along with collaborators Joel Bernier and Raymond Smith from Lawrence Livermore National Laboratory (LLNL).

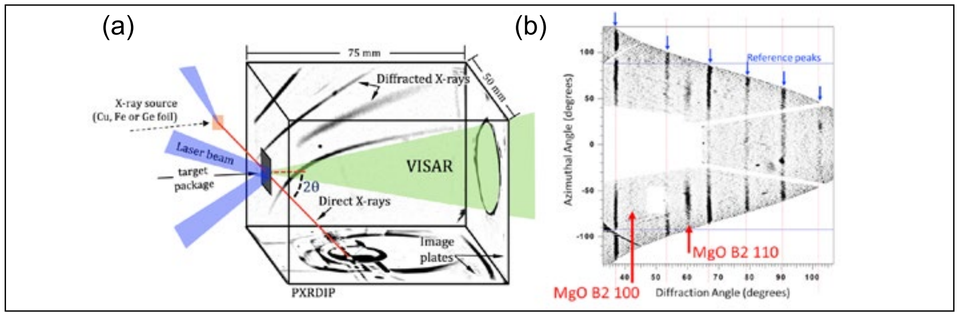

Figure 1. (a) Experiment geometry of the PXRDIP diagnostic at the OMEGA-60 laser system. (b) *In situ* X-ray diffraction pattern of ramp-compressed MgO projected into phi—d–spacing coordinates. Observed peaks demonstrate formation of the high pressure B2 phase of MgO.

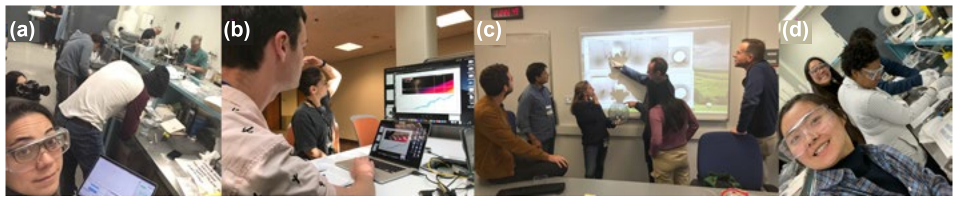

Figure 2. Paparazzi photos of JHU and LLNL students and collaborators from our first year.

Our aim is to contribute to the knowledge of the dynamic response of matter under ramp loading by developing and expanding tools to simulate and analyze *in situ* velocimetry and X-ray scattering measurements.[1-3] In this project, we focus on window materials of ramp compression experiments such as diamond and MgO, interrogating materials properties as a function of loading history. These studies not only will measure the dynamic response of materials at the lattice level, they will give insight into strength models and deformation mechanisms of these window materials.

This SSAP program provided partial support for three postdoctoral scholars, Drs. Nasim Eibagi, Vinay Rastogi, and Melissa Sims, who helped us launch projects on X-ray phase contrast imaging, ramp compression, and X-ray diffraction, respectively, and enabled training and research opportunities for multiple undergrad researchers. Our first year was focused on training with research projects on existing datasets and experiments at DCS, Cornell High Energy Synchrotron Source, and the University of Rochester Laboratory for Laser Energetics (LLE). Some highlights from our year included the graduation of undergraduate student Connor Krill who continued to collaborate with us on ramp compression tools while studying as a LLNL summer scholar under Drs. Suzanne Ali and Raymond Smith of LLNL (Figure 2b). Postdoctoral scholar Dr. Melissa Sims was awarded the prestigious National Science Foundation postdoctoral fellowship to carry out work that extends this year's projects into independent research under the mentorship of our team at JHU and Dr. Minta Akin at LLNL.

Scientifically, one highlight of our first year was a ramp compression study of single crystal MgO across the B1-B2 structural transition at the OMEGA-60 laser facility at the LLE. MgO is a promising window material for ramp compression due to its high transparency and moderate strength. The effect of the B1-B2 transition on window integrity, however, warrants further exploration. In this study, we carried out laser-driven ramp compression with *in situ* X-ray diffraction to study the crystallographic response.

The MgO sample was sandwiched between two single crystal diamond foils. Diamond served as an ideal material to couple laser energy and transmit pressure ramp compression waves. The diamond/MgO/diamond target was positioned on a Ta pinhole and then placed over the front of a Powder X-ray Diffraction with Image Plates (PXRDIP) box, which contains X-ray sensitive image plate detectors along the inner five walls (Figure 1a). The pressure history of the MgO sample and the time of peak compression is determined by a velocity interferometer system (VISAR) that accesses the rear of the target through an aperture at the back of the PXRDIP box (Figure 1a).

We used six high power laser beams focused to a 800-µm spot to dynamically compress 30-µm thick samples of single crystal MgO over eight nanoseconds and to pressures up to 600 GPa (6 million atmospheres). We employed temporal laser pulse shaping to ensure that the MgO sample experienced a progressively stronger applied pressure over time. Critically this ramp-compression approach allows materials to be examined at higher densities and lower temperatures than achievable through standard single shock compression experiments.

We found that single crystal MgO breaks up into a more powder-like assemblage across the B1-B2 transition (Figure 1b). This and future studies into the texture changes across phase transitions will inform our understanding of the time-dependent effects on properties such as material strength, phase transition mechanisms, and other barriers to atomic mobility. The subsequent effects on measurements of equations of state and optical properties will enable future experiments to be more accurately described.

References

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Accessing the Facility for Rare Isotope Beams' Ability to Provide Unstable Targets for Neutron Reaction Studies

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Graduate student Scott Essenmacher's PhD project focuses on capturing byproduct, radioactive material from a heavy-ion accelerator to produce targets for neutron reaction studies. With the help of postdoctoral researcher, Dr. Chirag Vyas, Scott is developing the necessary radiochemistry to allow stewardship science investigations with rare isotopes. Scott and Chirag have been supported since 2019 through the National Nuclear Security Administration's Stewardship Science Academic Alliances program in the group of Gregory Severin at Michigan State University (MSU).

The simulation models used in the Science-based Stockpile Stewardship program rely on accurate data to assess the viability of the nuclear stockpile.[1] One important piece of data, the neutron capture cross section (NCCS), defines the ability of various nuclei to absorb free neutrons, such as might be released in a nuclear detonation. Most nonradioactive nuclei have well-described NCCSs, but in a nuclear detonation many radioactive isotopes are formed which absorb neutrons in a relatively unpredictable fashion. The NCCSs for radioactive isotopes are very difficult to measure, because those isotopes have limited lifetimes and only can be produced in small quantities. Among the radioactive isotopes observed during underground weapons testing without a measured NCCS is vanadium-48 (^{48}V), which has 23 protons, 25 neutrons, and a half-life of about 16 days.[2] In addition to being unstable, ^{48}V is difficult to produce with high-enough purity to allow accurate NCCS measurements. So, how can a high-quantity and high-purity ^{48}V sample be made?

The new Facility for Rare Isotopes Beams (FRIB) at MSU will produce high energy beams of essentially any element on the periodic table. Unused portions of these beams are directed into a water-filled beam dump (Figure 1). Due to nuclear reactions between the beam and water, many different radioactive isotopes are produced. Useful radioisotopes can be collected from the water, isolated, and purified in a process called isotope harvesting.[3,4] For the case of ^{48}V, FRIB provides a unique route to a pure sample. Substantial quantities of chromium-48 (^{48}Cr), the radioactive parent to ^{48}V, can be harvested from the FRIB beam dump water. Over time, the harvested ^{48}Cr will generate a pure sample of ^{48}V, as ^{48}Cr decays into ^{48}V. With appropriate chemical processing, the ^{48}V can be prepared for neutron irradiation studies.

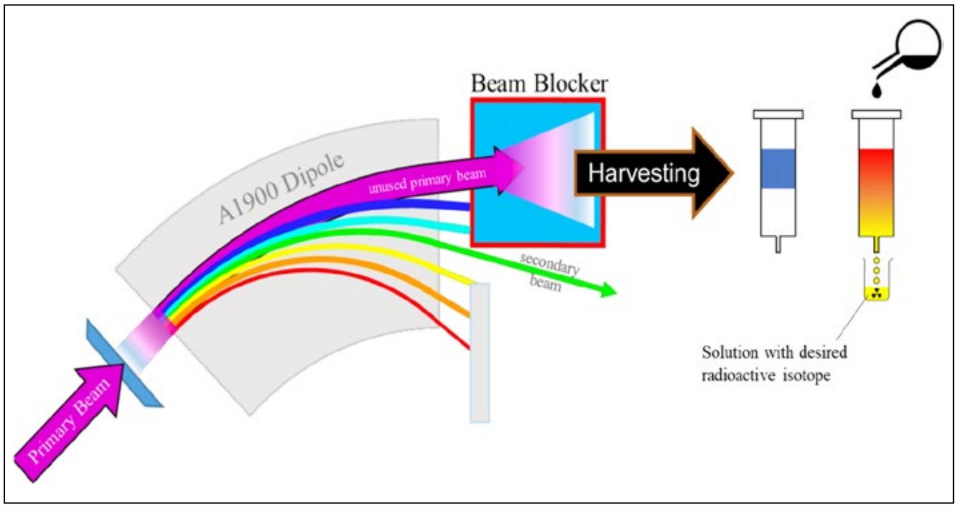

Figure 1. Graphic showing how isotopes will be produced and harvested from the FRIB facility at MSU with unused beam. Note that the secondary beam is the beam in which experimenters using the facility would be interested.

For safety and practicality reasons, research into $^{48}Cr/^{48}V$ harvesting starts with wet chemistry method development using nonradioactive chromium and vanadium. Research during the past year has shown that solutions can be made with non-radioactive chromium and vanadium in the same chemical form as the radioactive chromium and vanadium would be in the real beam dump,[5] which provides confidence that useful data can be obtained in studies with nonradioactive chromium and vanadium. Initial tests with chromium and vanadium using ion exchange media indicate that ^{48}Cr and ^{48}V will be removed efficiently from the beam dump system and can be coarsely separated from one another in a single step. Research into secondary separations currently is being conducted to refine the process and to improve the separation. Ultimately, this research aims to provide high purity ^{48}V to make neutron-reaction targets and to accurately determine its NCCS. In the future, many other unstable nuclei from FRIB may be harvested to support the Stewardship Science mission.

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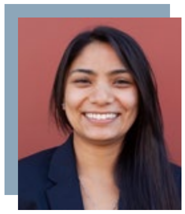
Years at SNL: August 2018-Present, **Degree:** PhD, Chemistry ✦ **SSAA Program:** 2014-2018, Washington State University



I work at Sandia National Laboratories (SNL) as a Senior Member of the Technical Staff in the Dynamic Material Properties group managed by Chris Seagle, also I am a Stewardship Science Academic Alliances (SSAA) alumni. I currently lead pre-compression work at both the Z-machine and at the hyper velocity gas-guns. The Z-machine is the world's largest and most powerful pulsed power machine which allows us to realize extreme states comparable to the deep interiors of Jupiter, Saturn and Neptune. Working at SNL gives me the opportunity to contribute to the field I love while also contributing to discoveries and breakthroughs much bigger than what I could accomplish anywhere else. The work we are doing is on the cutting edge of dynamic compression science and contributes in real ways to national security.

Collaborations and connections built through the SSAA program while I was a PhD student at Washington State University under the supervision of Professor Choong-Shik Yoo, significantly contributed to the privilege I now enjoy of working on this world-class and unique platform. I studied chemistries and phase transformations of various materials during my PhD work in Physical Chemistry. My work was funded through the SSAA project on Chemistry of Planetary Materials under Extreme Conditions. Part of my research also was funded through the CDAC program, a SSAA Center of Excellence. During Stewardship Science Academic Programs annual symposiums and other reviews/workshops, I was able to establish connections with people in various national labs which resulted in interviews for a postdoctoral position at three NNSA national laboratories, i.e., SNL, Lawrence Livermore National Laboratory, and Los Alamos National Laboratory. The opportunity to choose from three of the best laboratories is the outcome of the exposure I gained through SSAA. After one year as a postdoc at SNL, I was converted to my current position as a staff scientist.

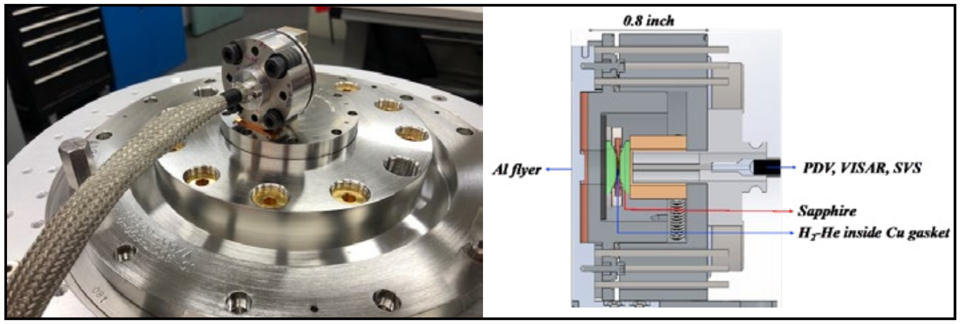


Figure 1. (Left) Assembled pre-compression cell in a stripline geometry for a Z experiment. (Right) Schematic of a pre-compression cell (2 inches wide and 0.8 inch tall). The fluid mixture of hydrogen-helium is captured inside the copper gasket placed in between two sapphire anvils.

> *"Collaborations and connections built through the SSAA program while I was a PhD student at Washington State University ..., significantly contributed to the privilege I now enjoy of working on this world-class and unique platform."*

Currently at SNL, I am studying the equation of state of pre-compressed H_2-He gas-mixtures under shock loading. Studying the pre-compressed mixtures of hydrogen-helium using plate impact techniques at the Z machine and the gas-guns provides a unique platform to obtain higher precision equation of state measurements than can be obtained from laser-shock studies. Pre-compression is an ideal method to study H_2-He gas mixtures, because it is the only way to obtain a miscible, homogeneous-fluid, initial sample due to the disparity in boiling points.

Our pre-compression cell, which is 2 inches in diameter (Figure 1), consists of two sapphire anvils in between which a copper gasket is placed where a compressed hydrogen-helium mixture at 25,000 psi is captured. A 100 µm thick quartz also is placed as a calibration standard. We use Al flyers at velocities up to 30 km/s (67,000 mph) to generate a shock that transits the sample. The diagnostics fielded in these experiments are velocimetry (VISAR and PDV) and Streaked Visible Spectroscopy (SVS). A series of experiments using the Z-machine and the gas-guns will enable the development of an experimentally-validated equation of state of the mixture.

Figure 2. Duwal holding a loaded pre-compression cell in front of the gas-loader.

Working at SNL not only has provided all the access to in-house facilities but also an opportunity to collaborate regularly across various other facilities, such as the High Pressure Collaborative Access Team, Dynamic Compression Sector at Argonne National Laboratories, and the Omega Laser Facility at the University of Rochester. Working in these facilities has enabled me to broaden my knowledge and skills while conducting research at some of the most advanced diagnostic and dynamic driver platforms in the world. The incredible team I work with teaches me new things every day, and as a result, I continue to make advances in my abilities and contributions to the field. I would definitely not be where I am today without the opportunities provided by the SSAA program and my education at Washington State University. I thank all the people who make this program possible!

Sarah Hickam, Los Alamos National Laboratory (shickam@lanl.gov)
Years at LANL: July 2019-Present **Degree:** PhD, Actinide Chemistry ✦ **SSAA Program:** 2017-2019, University of Notre Dame

I completed my PhD at the University of Notre Dame under the direction of Dr. Peter Burns as part of the Actinide Center of Excellence (ACE). The goal of my graduate work was to advance the understanding of actinide peroxide chemistry through the synthesis and characterization of actinide compounds, including a novel neptunyl triperoxide compound, and studies of actinide complexes in solution. My research also included the application of uranyl peroxide chemistry to dissolution of uranium materials like UO_2. My time working with actinide materials and characterizing solids and solutions using a variety of techniques, including Raman spectroscopy and X-ray diffraction, allowed me to develop a diverse skill set that I believe was useful as I sought opportunities in actinide science after graduation.

Support from the Stewardship Science Academic Alliances (SSAA) program during my last two years of my PhD was instrumental in providing opportunities that expanded my interests in plutonium science and stockpile stewardship that is central to my current professional goals. In particular, the program's focus on workforce development and providing graduate students like me the opportunity to do internships at the National Nuclear Security Administration (NNSA) national laboratories was crucial. Funding support provided by the SSAA program for an internship meant that I did not have to rely on open internship positions, and I had more freedom to reach out to scientists whose research I was interested in. My six-month internship at Los Alamos National Laboratory in the Chemistry-Actinide Analytical Chemistry group was invaluable and helped steer the direction of my post-graduate career by providing me with the experience working with plutonium and becoming familiar with the laboratory's mission. Being onsite at LANL gave me the opportunity to network and learn more about the diverse work being conducted at the laboratory as I planned for the next steps after my PhD.

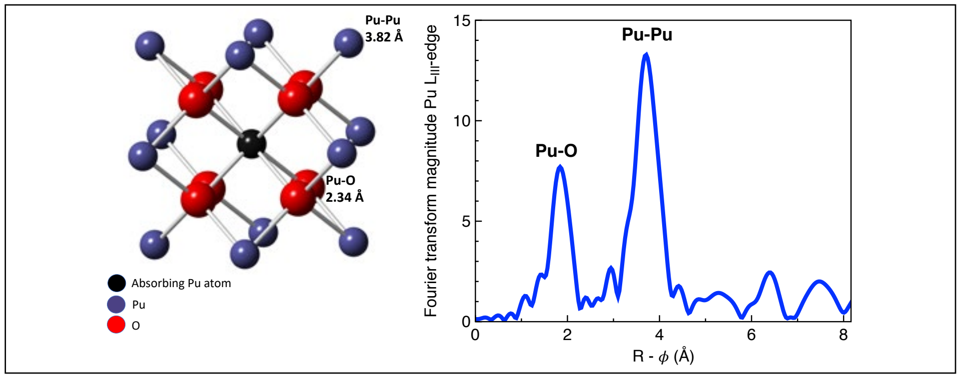


Figure 1. Extended X-ray absorption fine structure (EXAFS) spectra of a PuO_2 sample that was corroded from Pu metal (left) showing peaks that correspond to the Pu-O and Pu-Pu shells of the PuO_2 structure on the right.

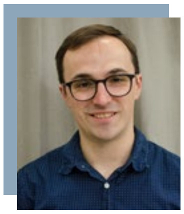
> *"...the program's focus on workforce development and providing graduate students like me the opportunity to do internships at NNSA national laboratories was crucial. Funding support provided by the SSAA for an internship meant that I did not have to rely on open internship positions, and I had more freedom to reach out to scientists whose research I was interested in."*

I wanted to continue my career at LANL because of the importance of the work and the exciting opportunities that exist for actinide science. Currently, I am a postdoctoral research associate in the Nuclear Materials Science (MST-16) group, whose mission includes "characterization of new and aged pit construction materials, development of technologies for advanced actinide materials analysis, and performance of actinide materials science investigations" (https://www.lanl.gov/org/ddste/aldps/materials-science-technology/nuclear-materials-science/index.php). The majority of my postdoctoral work is part of an NNSA-funded project that is led by the SLAC National Accelerator Laboratory and focuses on applying and developing advanced X-ray absorption spectroscopy (XAS) techniques for nuclear materials, with potential applications to fields such as nuclear forensics. My PhD experience in structural characterization and spectroscopy of actinide materials provided a good foundation to expand my skill set to include this technique, as XAS is a probe of the electronic and molecular structure of an element of interest in a sample.

An advantage of working at LANL is the accessibility to materials that are similar to those that might be found during nuclear forensics investigations, such as plutonium oxides formed by corrosion of Pu metal (Figure 1), which we can then study by XAS at synchrotron facilities including the Stanford Synchrotron Radiation Lightsource (SSRL at SLAC). XAS is sensitive to small changes in molecular structure that could be related to the history of the material, such as ambient temperature corrosion versus high temperature oxide formation. As part of the project, I also had the opportunity to organize a nuclear forensics workshop, which included presentations by scientists who are leaders in the nuclear forensics community. The ability to work with and learn from top scientists in the actinide field is one of the major privileges of working at a national laboratory such as LANL.

Cole D. Pruitt, Lawrence Livermore National Laboratory (pruitt9@llnl.gov)

Years at LLNL: December 2019-Present, **Degree:** PhD, Chemistry ✦ **SSAA Program:** 2018-2019, Washington University in St. Louis



I joined the low-energy nuclear community as a graduate student at Washington University in St. Louis where I finished my PhD in 2019. For the last stage of my doctoral research, I was supported by the Center for Excellence in Nuclear Training And University-based Research (CENTAUR) collaboration, a Stewardship Science Academic Alliances (SSAA) Center of Excellence for universities with graduate programs in nuclear experiments and theory. As a student, my research included experimental neutron total cross section work at Los Alamos National Laboratory (LANL) and new predictions for nuclear structure quantities including neutron skins (Figure 1) using a redeveloped Dispersive Optical Model (DOM) framework. As a postdoctoral fellow in the Nuclear Data and Theory group at Lawrence Livermore National Laboratory (LLNL), I am building a new generation of uncertainty-quantified nuclear optical potentials, a step toward improved reliability in nuclear scattering predictions.

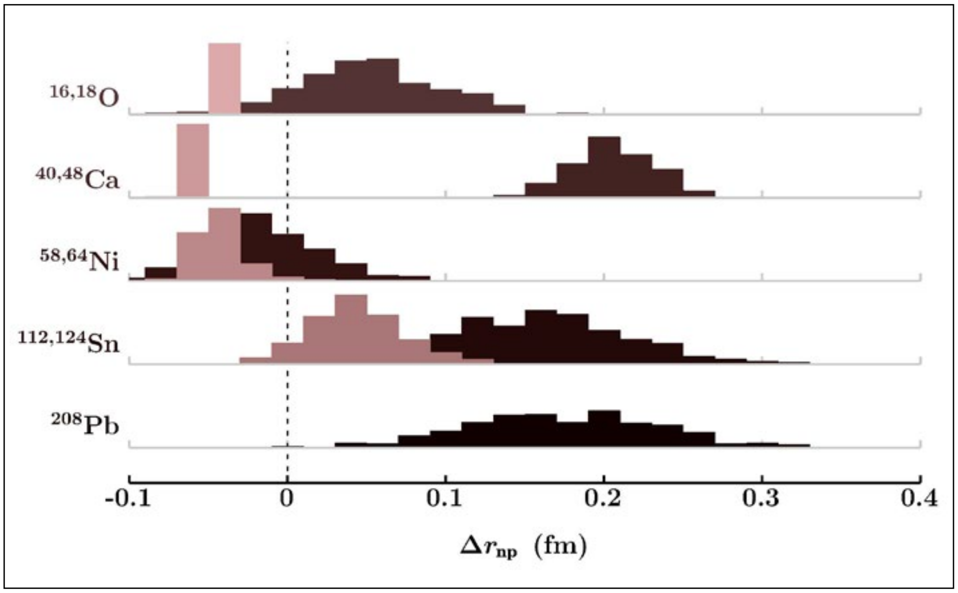


Figure 1.Neutron skin probability distributions from Markov-Chain Monte Carlo (MCMC) simulations for several closed-proton shell nuclides. The heights of each distribution have been arbitrarily rescaled to facilitate comparison. Reprinted from Pruitt et al., 2020, "Systematic Matter and Binding-Energy Distributions from a Dispersive Optical Model Analysis", Phys. Rev. Lett. 125:102501.

Today, the low-energy nuclear community faces both pressing infrastructure needs and renewed concerns about nuclear risk. With the last explosive nuclear tests conducted almost thirty years ago, many of the NNSA laboratories' employees are younger than the most recent test data. Very few employees with first-hand experience remain. At the same time, the national laboratories possess extraordinary tools to carry out stockpile stewardship and other long-term nuclear initiatives. Their success or failure hinges on an incoming generation of physicists, chemists, engineers, designers, and computer scientists, among others, becoming world-class experts in their technical domains and making the "national brain trust" available for policymakers. The core programs at the laboratories rely jointly on theory, experiment, and simulation in multiple subfields, and all of which depend on reliable, uncertainty-quantified data and algorithms. My research on reproducible, uncertainty-quantified, optical potentials is one thread in a larger tapestry. For me, the public- and community-service aspects of this work and the fact that my colleagues share an overarching commitment to reducing nuclear risk outweigh the opportunities in academia.

Talent development is a top priority at the national laboratories. Because the national security laboratories' stockpile stewardship mission has a many-decade horizon that is beyond the career of any single person, laboratory staff and management prioritize mentorship and professional development. As an example, as a technical postdoctoral fellow without policy experience, I have been encouraged to participate both in formal classes on applied deep learning techniques and in several laboratory-organized conferences about technology-policy issues, including whether the U.S. Nuclear Posture Review will be fit-for-purpose in the year 2030 and how new machine learning technologies may tip the balance of strategic stability. These talks and conferences afford personal interaction with experts on nuclear security issues, many of whom have international stature. LLNL encourages this kind of cross-pollination by providing postdoctoral fellows with the opportunity to devote 25% of their time to career development outside of their main research project. This culture of professional support is an important ingredient for building a more racially and economically diverse national security workforce, an effort that will require broader, sustained work in the academy as well. All of this matters for making the NNSA laboratories places that are worth working.

It should be mentioned that without the financial support from CENTAUR and SSAA, I would not have joined an NNSA laboratory. I met my current group leader, Jo Ressler, at a CENTAUR review session and my current project mentor, Jutta Escher, at a CENTAUR poster session later that year. I presented my work at the 2018 and 2019 Stewardship Science Academic Programs Review Symposia at which I met several staff and NNSA employees who encouraged me to consider laboratory opportunities. These were important connections for a graduate student with a background and priorities aligned for national laboratory work, but without extensive contacts across the NNSA laboratories.

David Bernstein (david-bernstein@uiowa.edu)
Degree in Progress: PhD, Plasma Physics, University of Iowa ✦ **Advisor:** Dr. Scott D. Baalrud; **SSAA:** 2019-Present

Research Topic

Simulation and Theory of the Friction Force on Test-particles in Dense (Strongly-Coupled) and Strongly-Magnetized Plasmas

Research Responsibilities

As a member of the Center for Advanced Nuclear Diagnostics and Platforms for ICF and HED Physics at Omega, NIF, and Z, led by Dr. Richard Petrasso at Massachusetts Institute of Technology, my responsibility is to understand the fundamental physics of macroscopic transport in strongly-magnetized and strongly-coupled plasmas through the friction force on test-particles. More accurate transport models are then developed, which are used in codes developed at the Center or compared directly with experiments. I study the friction force because it describes the particle-plasma interactions that dictate microscopic particle dynamics responsible for macroscopic transport such as diffusion or thermal relaxation rates.

My research incorporates a blend of theory and simulation work. For the computational components, I conduct first-principles molecular dynamics simulations run on high-performance computing clusters and analyze the data with my own post-processing methods. I then compare these outputs with theoretical predictions. When discrepancies between theory and simulations arise, I attempt to understand why they occur and to resolve them. My research responsibilities include disseminating my work and results through talks at conferences and publishing in peer-reviewed journals.

Benefits of SSAA

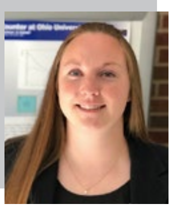
The Stewardship Science Academic Alliances (SSAA) program has provided unique opportunities to connect with other researchers. These connections occur through interactions within the Center of Excellence and at the annual SSAP symposiums. I would not have had these opportunities were it not for the SSAA program. At the symposiums, I have had the chance to connect with researchers at various national laboratories with whom I hope to engage for a postdoctoral fellowship.

National Laboratory Experience

I spent two summers at Los Alamos National Laboratory (LANL) working with our collaborator Dr. Jerome Daligault. These summers were formative for my training as a researcher. Working with both my advisor, Prof. Scott Baalrud at the University of Iowa, and Dr. Daligault provided me with multiple points of view for approaching theoretical and computational plasma physics. Working at LANL exposed me to the exciting work and environment that the national laboratories have to offer. Because of the positive experience I had at LANL, I have chosen to pursue a postdoctoral position at a national laboratory. I have found the SSAA program to be an excellent means for making professional connections that I would not have had if I were not part of this organization. Overall, these connections and my time at LANL have positively and majorly impacted my career.

Kristyn Brandenburg (kb851615@ohio.edu)
Degree in Progress: PhD, Nuclear Physics, Ohio University ✦ **Advisor:** Dr. Zachary Meisel; **SSAA:** 2017-Present

Research Topic



Neutron Detection from (alpha,n) Reactions Relevant for Energy Generation and Diagnostics from Nuclear Fission and Nuclear Fusion

Research Responsibilities

I am a part of a team of low energy nuclear physicists who perform reaction measurements at the Ohio University Edwards Accelerator Laboratory. I have designed and commissioned a new detector for our lab that has special capabilities to measure with high precision cross sections relevant to special nuclear materials, molten salt reactors, and inertial confinement fusion. For example, alpha particles are emitted from fissile materials and can interact with surrounding materials to produce neutrons via the (alpha,n) reaction. Problems can arise when additional neutrons enter the surrounding environment causing potential damage to detector systems and can further complicate analyses due to large neutron backgrounds. Accounting for the neutron flux can be done if the cross sections of the reactions involved are known. However, many of these reactions have not yet been measured. Additionally, several prior measurements of (alpha,n) reactions do not agree with each other or with existing theory. The detector that I developed is being used to measure the reactions of interest, and due to its specific design, will provide cross sections with low uncertainty.

Benefits of SSAA

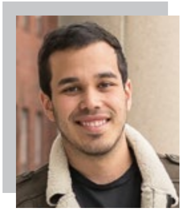
Through the SSAA program, I have been able to grow as a researcher by traveling to conferences and talking with other scientists in fields similar to and different from my own. Specifically, the poster presentation sessions gave me an opportunity to share my work and to cultivate skills in discussing and answering questions from experts in the field. I am thankful to the SSAA program for funding my research and for providing me the experience to learn more about national laboratories.

What Students Considering SSAA Should Know

Future students, the SSAA program brings together a diverse set of researchers from many universities and national laboratories. You will have opportunities to develop your skill set through communications with them that one day could lead you to your forever career. We are very fortunate in this sense, and I hope that you will get as much out of the SSAA program as I have.

Ian Colliard (colliari@oregonstate.edu)

Degree in Progress: PhD, Inorganic Chemistry, Oregon State University ✦ **Advisor:** Dr. May Nyman ✦ **SSAA:** 2017-Present



Research Topic

Solution and Solid-State Characterization of Actinides and Actinide-metal Oxo Species

Research Responsibilities

My research looks into the dissolution and formation of actinide oxides from aqueous solutions, in particular the tetravalent series (Th^{IV}, U^{IV}, Pu^{IV} or Ce^{IV}) as a surrogate for plutonium. With this scheme we try to crystallize out fragments of the oxide lattice in order to understand the formation mechanisms. Furthermore, we can test the effect that other metals, such as lanthanides or other fission products, can have on metal oxide growth. We then look at the new actinide-oxo species through a single crystal diffractometer to determine the size, shape, and packing of the new structure. After which, we characterize any new properties. One big surprise is the controlled supramolecular assembly of the metal-oxo species in solution, which open the field to some interesting chemistry.

Benefits of SSAA

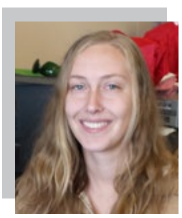
Being a part of the SSAA program and the Actinide Center for Excellence community led by Dr. Peter Burns at the University of Notre Dame, has been a very welcomed surprise. The instrumentation available and the techniques one can learn, especially with people at the top of their field, is very helpful. Being such a close-knit community, people in the same field tend to know each other which makes it easier to start conversations.

National Laboratory Experience

The program and the community have a lot to offer. People are committed to the students making sure we have what we need to conduct our research and to learn the necessary techniques. They also look to make sure the students have tools to move on to the next step whether it's to a national laboratory or to academia.

Samantha Couper (samantha.couper@utah.edu)

Degree in Progress: PhD, Geophysics, The University of Utah ✦ **Advisor:** Dr. Lowell Miyagi ✦ **SSAA:** 2016-Present



Research Topic

Microstructures and Deformation Mechanisms Driving Lattice-Preferred-Orientation of Low Symmetry Earth Materials at Extreme Pressures and High Temperatures Under Low Strain Rates (~10^{-4}).

Research Responsibilities

In the laboratory, I am responsible for tracking inventory and preparing, aligning, and loading diamond anvil cells. These are used for *in situ*, synchrotron experiments at high pressure (at Lawrence Berkeley and Argonne National Laboratories) and often temperature in a radial diamond anvil cell. I act as the on-site lead and teach fellow students or collaborators the process. I am responsible for Rietveld refinement of powder diffraction patterns collected at the synchrotron and run plasticity models against these results to interpret possible deformation behavior and deformation mechanisms active within the samples.

Benefits of SSAA

I am a part of the Chicago/DOE Alliance Center (CDAC) led by Dr. Russell Hemley at the University of Illinois at Chicago, which seeks to advance high pressure and temperature studies for application to Stockpile Stewardship science. My PhD research has been funded primarily through CDAC, and I have been fortunate to receive shifts at the Advanced Photon Source (APS) during each cycle. The consistent access to the beam was key in teaching me the ability to independently run experiments and to learn new techniques, such as dynamic compression. I have been able to collaborate with beamline staff at APS which has helped me develop professional relationships and has provided access to internship and networking opportunities.

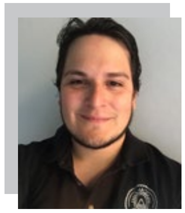
National Laboratory Experience

Through CDAC, the SSAA program provided first-hand access to the work and research environment of the national laboratories. I had the opportunity to intern at Lawrence Livermore National Laboratory (LLNL) during the summer of 2019, and using LLNL facilities, I could model the grain-to-grain interactions between multiple Earth material phases in a single sample. Our university laboratory facilities are limited to models that can compare relationships between two grains but cannot model microstructural interactions throughout the entire sample. Therefore, my internship at LLNL provided both an essential component of my dissertation and a more thorough understanding of the physics of multiphase materials.

Support by my mentors at APS and LLNL has provided skills and networking and friendship opportunities that I would not have had access to without the Stewardship Science Academic Alliances. The combination of world-class facilities, scientists, and the positive work environment made me seriously consider a career at a national laboratory, and I now have accepted a postdoctoral position at Los Alamos National Laboratory (LANL). The connections and knowledge I gained at APS and LLNL resulted in a competitive resume and the flexibility to choose a program that would be the best fit for my interests. Before my involvement with CDAC, I did not know about stockpile stewardship, and I certainly had not entertained a career at a national laboratory. I am thankful to the program for opening these doors and look forward to continued collaborations with national laboratories made possible through the SSAA program.

Marco Jose Echeverria (marco.echeverria@uconn.edu)

Degree in Progress: PhD, Materials Science and Engineering, University of Connecticut ✦ **Advisor:** Dr. Avinash Dongare ✦ **SSAA:** 2018-Present



Research Topic

Fracture Behavior of Shock-Loaded Materials at the Atomic Scale

Research Responsibilities

As a member of the Center for Research Excellence on Dynamically Deformed Solids (CREDDS) led by Dr. Michael Demkowicz at Texas A&M University, my research aims to investigate the deformation and failure behavior of multiphase, metallic materials under shock loading conditions at the atomic scales. The response is observed to be determined by the loading conditions (shock duration and velocity) that change the shock pressures and strain rates of the loading experienced by the material and the microstructure of the metal. As part of the Computational Materials and Mechanics Group at the University of Connecticut, my goal is to develop computational methods to mimic the shock-loading conditions as observed using laser-shocks. My work aims to characterize the evolution of defect structures (dislocations, twins) that are generated to guide experiments on the relevant mechanisms that operate during the various stages of deformation and failure. To investigate the importance of the microstructure, the simulations are carried out for various loading orientations and interfaces that are observed in the experimentally-synthesized microstructures. This gives a crucial insight into understanding the role that heterogeneities play in the dislocation transport through interfaces and which of these govern the fracture mechanism known as spall failure. Exploring the spall phenomena is key to enabling the tailoring of damage-resistant materials that can be used in applications where extreme environments are the norm.

Benefits of SSAA

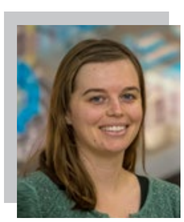
The Stewardship Science Academic Alliances (SSAA) program provides multiple networking opportunities that have greatly impacted my research. Not only is collaboration with graduate students from other universities possible, but collaboration with professors and national laboratory staff who conduct cutting edge research also is possible. This relationship has provided important insights into my molecular dynamics simulations through years of knowledge that can be accessed by these collaborations.

National Laboratory Experience

One benefit I received from the SSAA program was the networking opportunity with scientists from the Lawrence Livermore National Laboratory (LLNL) at the Stewardship Science Academic Programs symposium in Albuquerque, New Mexico. That interaction gave me the opportunity to participate in summer internships at LLNL in 2019 and 2020, where we investigated another interface phenomenon: ejecta formation. My molecular dynamics simulations have helped the team understand the importance of interface morphology and loading conditions in investigating the role that microstructure plays in ejecta formation. The collaborations formed and the knowledge learned working with scientists from the national laboratories are extraordinarily beneficial.

Dana Zimmer (dmzimmer@eng.ucsd.edu)

Degree in Progress: PhD, Engineering Physics, University of California, San Diego ✦ **Advisor**: Dr. Farhat Beg ✦ **SSAA**: 2019-Present



Research Topic

Formation of a Millimeter-Scale, Field-Reversed Configuration using an Auto-Magnetizing Liner

Research Responsibilities

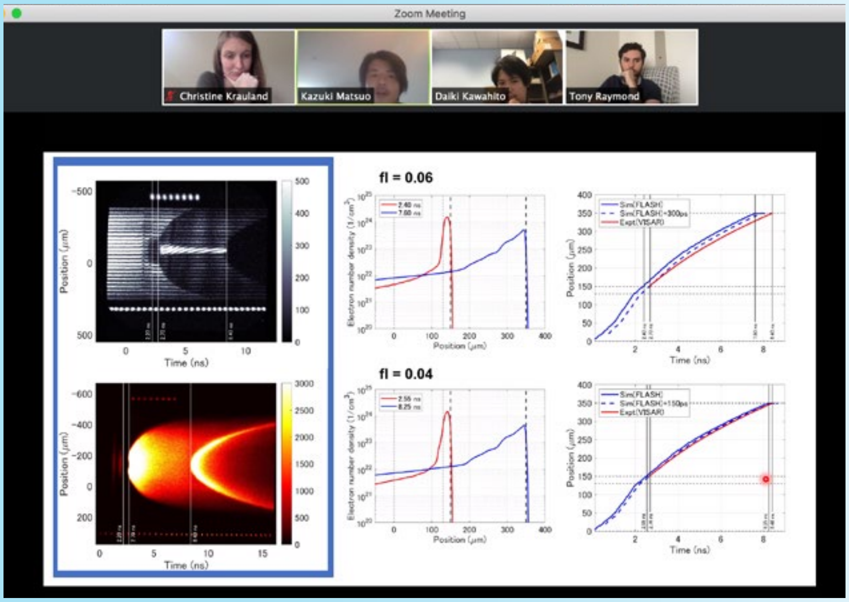
As a second-year graduate student under Farhat Beg at the University of California, San Diego, I have had the good fortune of taking part in several illuminating research opportunities that were made possible by funding from the Stewardship Science Academic Alliances (SSAA) programs. In the summer of 2019, I interned at Lawrence Livermore National Laboratory studying neutron production from collisionless shocks through the analysis of the neutron time-of-flight diagnostic data with the Astrophysical Collisionless Shock Experiments in the Laboratory collaboration. Facilitating our understanding of shock formation in extreme astrophysical environments such as supernovae remnants, this unique project utilizes the world-class National Ignition Facility to recreate these exceptional conditions in a controlled, laboratory setting. In the summer of 2020, I was able to intern remotely (due to COVID-19 restrictions) with Sandia National Laboratories studying current loss through velocimetry analysis in the Z pulsed power machine. This project provided a remarkable opportunity to advance the performance of the Magnetized Liner Inertial Fusion experiments, one of the leading candidates for developing the capability of break-even fusion energy.

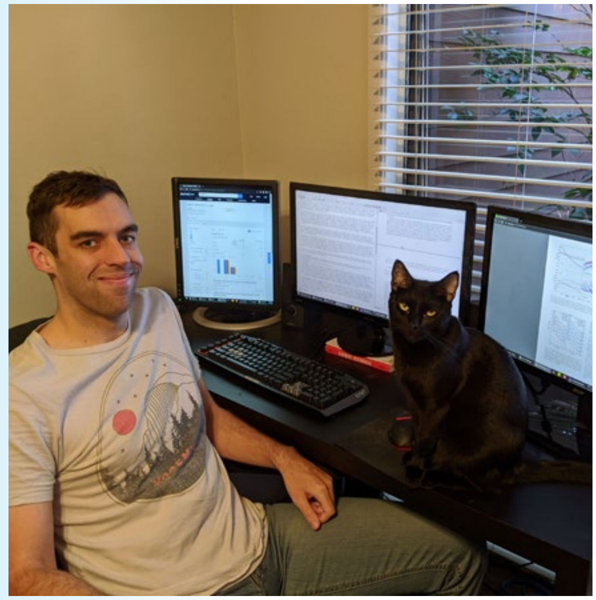
Benefits of SSAA

Beyond my internships at our outstanding national laboratories, the SSAA program has facilitated my participation in several enriching experiences with the Center for Matter Under Extreme Conditions (CMEC) that have been highlights of my graduate education thus far. During the summer of 2019, I attended the High Energy Density Science Summer School (HEDSSS), a two-week lecture series targeted toward graduate students and postdoctoral fellows that covered a wide range of topics relevant to high energy density science, such as material science in extreme conditions and ultra-intense laser-matter interactions. Furthermore, in early 2020, I traveled to Rochester, New York to participate in a long day of experiments on the OMEGA-EP laser at the Laboratory for Laser Energetics. Directed by Dr. Chris McGuffey, these experiments heated a silicon target to warm dense matter conditions by employing the short-pulse lasers to generate high-intensity ion beams which were directed at the target.

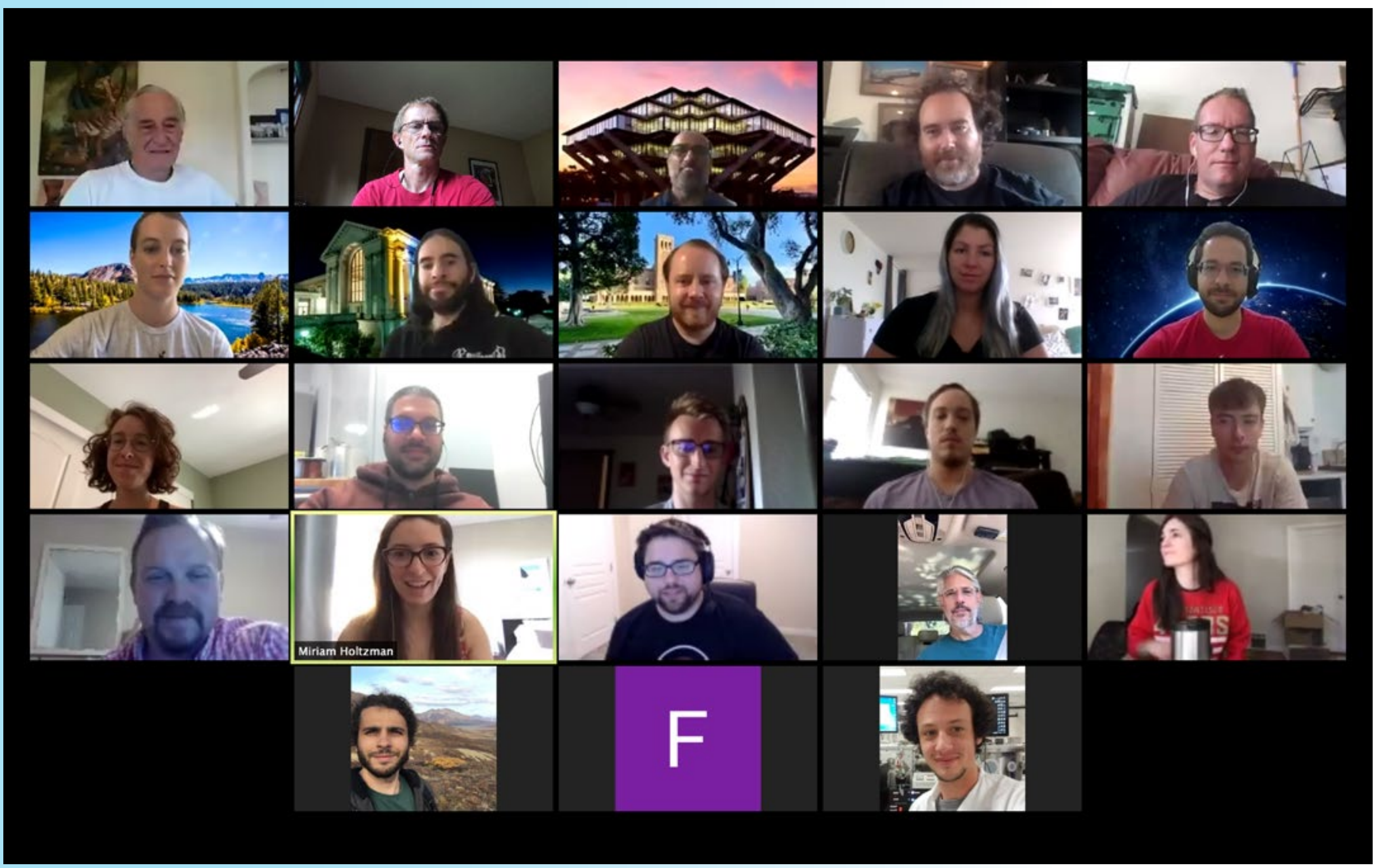
What Students Considering SSAA Should Know

As a direct result of funding from SSAA, I have had the freedom to engage in academic exploration of several distinct research topics and to make many connections with personnel from the national laboratories. It was expressly through these relations that I have now found a topic for my PhD research that inspires and stimulates me.





Research Looks Different This Year!



High Energy Density Laboratory Plasmas

Pulsed Power Driver to Generate and Measure HED States

Idaho State University ✦ PI: Dr. Jon Stoner (stonjon@isu.edu)

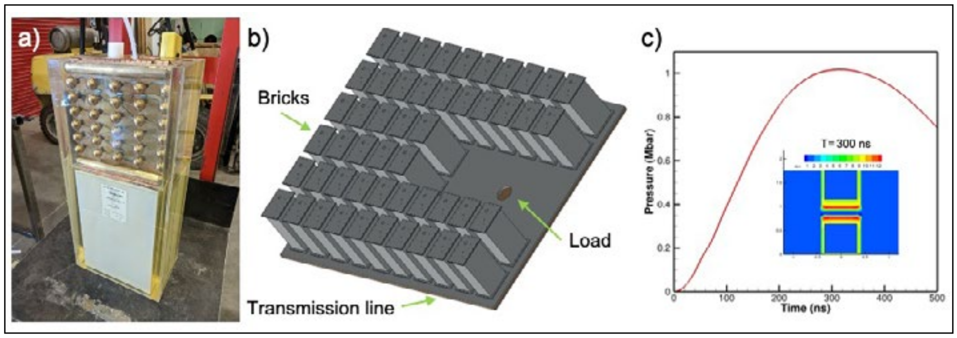


Figure 1. (a) Cinco building block, the 100 kA brick. (b) 50-brick Cinco generator with strip-line quasi-isentropic compression load. (c) Performance of fully configured Cinco showing the compression of copper to 1 Mbar (100 GPa).

Figure 2. Graduate student Travis Bejines and IAC Engineer Brian Berls assembling the 4-Brick Cinco generator. This device, capable of 320 kA, will allow the validation of all key components, a necessary step before building larger Cinco devices with ramp compression loads.

The magnetically-driven, quasi-isentropic compression technique was first developed on the Z accelerator at Sandia National Laboratories. This technique has yielded revolutionary improvements in the accuracy of material properties in the multi-Mbar (hundreds of GPa) pressure regime. Critical to the Stockpile Stewardship Program is the understanding of dynamic material properties in this high-pressure regime.

At the Idaho State Accelerator Center (IAC) the portable and low-cost driver called Cinco (Figure 1) is being developed to generate these desired states of matter. Although not capable of the ultra-high pressures of a large facility, Cinco would have greater shot-throughput and would be more economical to operate in a university environment. This work is being performed by Idaho State University PhD student Travis Bejines. The design uses an efficient current-adder configuration of capacitor-switch elements. Cinco, when fully configured, can produce a peak current of 5 MA which, in turn, produces a peak quasi-isentropic pressure drive of 1 Mbar (100 GPa). Cinco also can produce shock states of up to 4 Mbar (400 GPa) using magnetically-driven, hypervelocity flyer plates.

The Cinco project currently is in its third year. The plan for development of the Cinco generator first involved the development of the capacitor-switch unit called the brick. Over 200 experiments have been performed on the single-brick fixture. Using these building blocks, a 4-brick version of Cinco then was constructed (Figure 2). This device currently is being validated through numerous tests and comparisons to simulation. This step allows confidence in proceeding to the development of larger Cinco machines capable of driving dynamic materials' loads. The current effort is to construct a 10-brick Cinco with a 1.2 MA, 100 kbar (10 GPa) ramp compression load. One interesting campaign on this machine, and a subject of Bejines' thesis, will be driving a zirconium sample to observe the $\alpha \rightarrow \omega$ phase transition.

Through possible continuation funding for a fourth year, a full Cinco device consisting of 50 bricks could be fabricated. This portable, 50-brick Cinco could be located at the appropriate X-ray light source. One option for this is the Matter in Extreme Conditions (MEC) station on the Linac Coherent Light Source (LCLS) at the SLAC accelerator, among others. This would allow X-ray diffraction (XRD) experiments to be performed on compressed samples, thus allowing the study of *in situ* dynamic properties of materials at a wide variety of high-pressure conditions. The results would open many new possibilities of high energy density physics in the areas of equation of state, phase transitions, and warm dense matter. In support of the High Energy Density Laboratory Plasmas program, this would enable the training of many students in dynamic material science, an area important to the National Nuclear Security Administration's mission in stockpile stewardship science.

Seeding and Evolution of Magnetohydrodynamic Instabilities of a Metal Surface Driven by Intense Current

University of New Mexico, University of Nevada, Reno, and Virginia Polytechnic Institute and State University ✦ PIs: Dr. Mark Gilmore (mgilmore@unm.edu), Dr. Bruno Bauer (bbauer@physics.unr.edu), and Dr. Bhuvana Srinivasan (srinbhu@vt.edu)

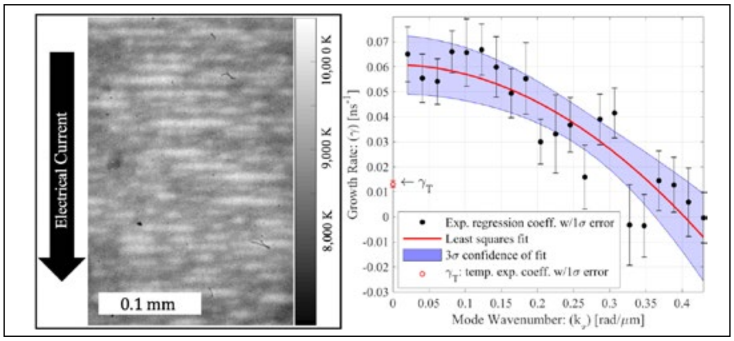


Figure 1. Left: ETI perturbations are seen in the aluminum-6061 surface temperature (from a 3-μm/3.5-ns-FWHM-resolution image). Right: ETI exponential growth rate vs perturbation wavenumber.

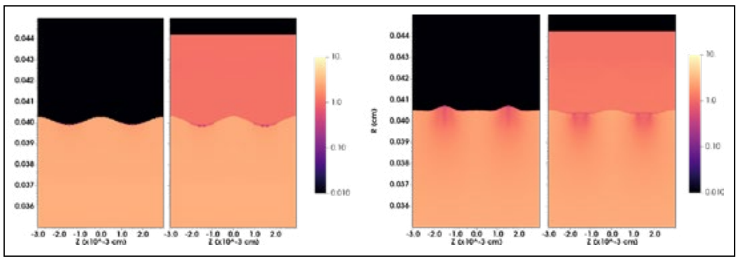


Figure 2. Ares simulations of current-driven 0.8-mm-diameter aluminum-6061 rods with and without a 41-μm-thick dielectric coating. Left pair of plots: The surface of both aluminum rods initially contains a 5-μm-amplitude perturbation, as seen in the initial density (g/cm^3). The leftmost plot of the pair shows the uncoated aluminum rod, whereas the rightmost displays the coated case. Right pair of plots: Near the onset of phase change (at ~50 ns), the density (g/cm^3) shows smaller aluminum surface perturbations for the coated rod (right) than for the uncoated one (left).

The formation and evolution of instabilities on a metal surface pulsed by an intense current is of great importance to fundamental high energy density (HED) physics and to a wide variety of applications. Thanks to support from the High Energy Density Laboratory Plasmas program since 2018, three faculty members and six graduate students at the University of New Mexico, University of Nevada, Reno, and Virginia Polytechnic Institute and State University are investigating this exciting topic with state-of-the-art experiments and computer modeling in collaboration with researchers at Sandia National Laboratories (SNL), Los Alamos National Laboratory (LANL), and Lawrence Livermore National Laboratory (LLNL). Extreme current densities (e.g., 10^{12} A/m^2) are common in pulsed power experiments such as those at SNL on Magnetized Liner Inertial Fusion (MagLIF). A sequence of interconnected instabilities limits the results achieved, such as the thermonuclear conditions useful for Stockpile Stewardship. This project focuses on the earliest current-driven instability in metal, the electrothermal instability (ETI), and its connection to later magnetohydrodynamic (MHD) instabilities.

To examine the instabilities experimentally, graduate students Trevor Hutchinson (postdoctoral researcher at LLNL at the time of printing), Maren Hatch, and Aidan Klemmer pulse mm-diameter metal rods with mega-ampere current. Using a suite of advanced diagnostics, they examine the evolution of the metal, nanosecond by nanosecond. On such fast timescales, heat from the current cannot dissipate, and the metal temperature quickly rises to much larger than its boiling point. The ETI causes ‘rippling’ of the current density and 1,000 K temperature variations. Direct observation of thermal perturbations together with their exponential growth was achieved for the first time[1] (Figure 1) and was highlighted by APS Physics Buzz.[2] Subsequently, the surface expansion velocity of dielectric-coated metal driven by intense current was measured for the first time, using Photonic Doppler Velocimetry (PDV) at the SNL Mykonos facility.[3]

The explosion and instability of metal driven by intense current is very challenging for computational codes to accurately model, as the metal traverses many states of matter, from solid to liquid, gas, warm dense matter, and plasma. Detailed computer simulations of the experiments are being performed by graduate student Seth Kreher, using the LANL FLAG code, and by graduate students Robert Masti and Matthew Carrier, using the LLNL Ares code. These multi-physics, multidimensional, arbitrary Lagrangian-Eulerian (ALE) MHD codes are well suited for studying ETI (Figure 2).[4]

The novel PDV surface expansion velocity measurements are proving vital for benchmarking numerical modeling and discriminating between different material-data tables for multi-thousand-degree, low density aluminum. Better agreement is being achieved between the computations and the experimental data, developing understanding of how to model metal driven by intense current, and increasing the predictive capability of numerical simulation.

To understand from which initial conditions ETI grows, the most recent experiments explicitly track microscopic details in the metal from machining through self-emission at high temperatures. The data enable evaluation of the influences of metallurgical defects, surface topography, and crystallographic grain boundaries on instability development.[5] Moreover, the nonuniform heating around deliberately machined hemispherical surface pits is being measured and compared with three-dimensional MHD simulations.[6]

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[1]T.M. Hutchinson et al., “Experimental Observation of the Stratified Electro-Thermal Instability on Aluminum with Thickness Greater Than a Skin Depth,” Phys. Rev. E 97, 053208 (2018).

[2]http://physicsbuzz.physicscentral.com/2018/07/what-happens-when-you-plug-wire-into.html

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[5]T.M. Hutchinson et al., “On the Relative Importance of the Different Initial Conditions That Seed the Electrothermal Instability,” (in preparation).

[6]E.P. Yu et al., “Use of Hydrodynamic Theory to Estimate Electrical Current Redistribution in Metals,” Phys. Plasmas 27, 052703 (2020).

"This is where the High Energy Density Laboratory Plasmas (HEDLP) program played an important role in my research, providing funding and support for a long journey from theoretical ideas to the U.S. patent on Otto and Diesel Cycles Employing Spinning Gas."

— Dr. Vasily Geyko
Lawrence Livermore National Laboratory

"With the HEDLP program, I have had the opportunity to interact with prominent scientists in this field from academia and national laboratories, compelling me to strongly consider a career in high energy density science."

— Krish Bhutwala
University of California, San Diego

"The HEDLP program has given me the opportunity to become involved with MagLIF and to use my research to contribute to the advancement of this fascinating approach to inertial fusion."

— Kyle Carpenter
University of Nevada, Reno

Vasily Geyko, Lawrence Livermore National Laboratory (geyko1@llnl.gov)
Years at LLNL: March 2018-Present ✦ **Degree:** PhD, Plasma Physics ✦ **HEDLP:** 2013-2017, Princeton University

During my doctoral research at Princeton University under the supervision of Professor Nathaniel Fisch, I worked on a number of different problems. Among them was a problem of energy deposition and manipulation in plasma with varying parameters such as density or temperature. This type of plasma can be found, for example, in a Z-pinch, a device in which a plasma column is compressed by the generated azimuthal magnetic field. Apart from the thermal energy of plasma particles, there are other mechanisms for energy deposition, in particular, energy of embedded plasma waves, turbulence, or rotation. The latter was of interest for me, as rotation is a very robust phenomenon due to the conservation of angular momentum.

To improve my intuition on the complicated physics of a spinning plasma, I first posed a spinning neutral gas problem in the thermodynamic limit. Despite the apparent simplicity of the problem, I discovered some fascinating things. I found reduced compressibility caused by the additional degree of freedom associated with rotation. I then was able to pose an inverse problem to determine gas constituents through measurements of external parameters only. Apart from the academic interest, there could be an application in determining what is inside a container if it is unsafe to open. It also was revealed that the use of a spinning gas in thermodynamical cycles could improve their efficiency by several percent—a number that might be significant if the standard efficiency is only 20-30%. Moreover, as a spinning gas is compressed, a radial temperature differential is formed creating a hot spot in the center of the cylinder which further improves the efficiency of the spinning-gas-based thermal cycle. This is where the High Energy Density Laboratory Plasmas (HEDLP) program played an important role in my research, providing funding and support for a long journey from theoretical ideas to the U.S. patent on Otto and Diesel Cycles Employing Spinning Gas.

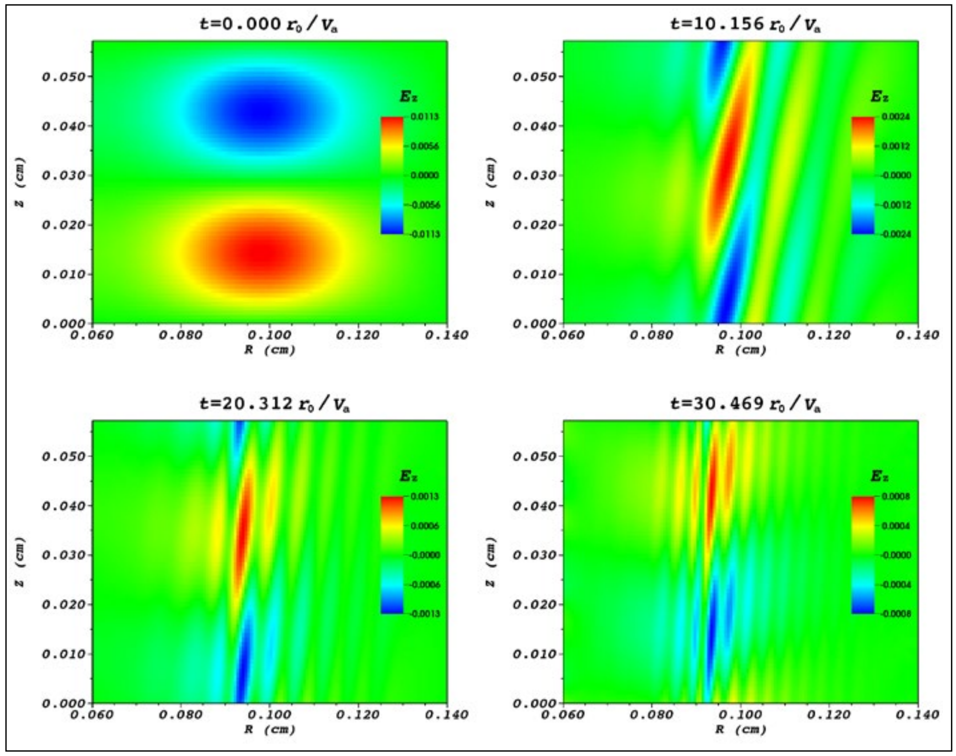


Figure 1. Snapshots of the time evolution of the seeded perturbation in a SFS Z-pinch. Each plot illustrates spatial distribution of the normalized axial electric field of the perturbation in the RxZ plane. Flow shear stretches and smears the perturbation, so that no exponential growth is observed, and the pinch is stabilized against a linear mode of a given axial mode number r_0k_z=10, where r_0 is the pinch characteristic radius.

Inspired by the research done at Princeton University, I was searching for a career with the National Nuclear Security Administration's national laboratories. Currently I am working at Lawrence Livermore National Laboratory (LLNL) on instabilities in the sheared flow stabilized (SFS) Z-pinches. The concept relies on the idea that a flow shear can smear out spatial structures of the unstable modes and lead to the stabilization of the pinch. Numerical simulations commonly used in the community to approach this problem either are fluid-based or fully-kinetic. The fluid-based simulations are missing some important kinetic effects related to the finite size of the ion gyro orbit, and the fully-kinetic simulations are very slow and inefficient if a huge scan of parameters is needed. It was suggested that a gyrokinetic approach instead could be used, since it retains kinetic physics and provides significant speed-up compared to fully-kinetic codes. I adopted the LLNL gyrokinetic code, COGENT, that was designed initially for tokamak applications and investigated stability properties of SFS Z-pinch plasmas at different parameters. Whereas I could confirm in the simulations that some linear modes indeed can be stabilized by the flow shear (Figure 1) with the values of shear reported in recent experiments, no global stabilization has been observed. Interestingly, the growth rate of the modes and their response to the flow shear strongly depend on the pinch radial density and temperature profiles, and it is speculated that a nonlinear kinetic mechanism might be responsible for the global stabilization. In any case, the problem remains open, and more advanced numerical tools are required to perform further investigation.

In conclusion, the HEDLP program provided a great opportunity for me to develop necessary skills, conduct the research of truly exiting problems, spread the results to the scientific community, and get valuable feedback. It aided considerably in the pursuit of my career at Lawrence Livermore National Laboratory.

Krish Bhutwala (kbhutwal@eng.ucsd.edu)

Degree in Progress: PhD, High Energy Density Physics, University of California, San Diego ✦ **Advisor:** Dr. Farhat Beg ✦ **HEDLP:** 2017-Present

Research Topic

Proton Transport and Energy Deposition in Warm Dense Matter

Research Responsibilities

I am conducting particle-in-cell simulations to investigate proton stopping power and energy deposition in warm/hot dense matter conditions. Warm dense states of matter lie at the very intersection of condensed matter physics and plasma physics, characterized by temperatures of 1-100 eV and densities within two orders of magnitude of solid density. In this regime, the electron thermal energy is on equal footing with both the Coulomb energy between electrons and nuclei and the Fermi energy of the system, convoluting many properties of the system.

Proton stopping and energy deposition in warm dense matter proves vital in certain schemes of inertial confinement fusion, where laser-accelerated protons and ions impart their energy into a pre-compressed deuterium-tritium capsule. Proton stopping in cold matter as well as in hot plasmas has been well-investigated, but that in warm dense matter is not as well-known. I simulate proton stopping in warm dense matter using an ad-hoc stopping model with contributions from both bound and free electrons, the proportions of which are gained from the temperature- and density-dependent ionization state of the material. Using this model, we can investigate the dynamic evolution of material Ohmic heating and proton beam transport from current densities high enough to heat the material to warm dense states.

Benefits of HEDLP

Not only has my research been supported through an HEDLP grant, but also I have been fortunate enough to gain hands-on training and experience at several prominent NNSA laser facilities across the country, including the Laboratory for Laser Energetics (Rochester, NY) through National Laser Users' Facility, the Jupiter Laser Facility at Lawrence Livermore National Laboratory (Livermore, CA), and the Office of Science Matter in Extreme Conditions (MEC) End-Station at the SLAC National Accelerator Laboratory (Menlo Park, CA). With the HEDLP program, I have had the opportunity to interact with prominent scientists in this field from academia and national laboratories, compelling me to strongly consider a career in high energy density science.

What Students Considering HEDLP Should Know

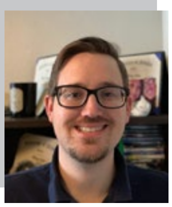
Students should understand that one of the fundamental objectives of the HEDLP program is to train students, the future generation of scientists. If you are part of the program, they genuinely are invested in your advancement! Science is always a team effort, so participating in and interacting with the scientific community is in not only your but everyone's best interest.

Kyle Carpenter (kcarpenter2@unr.edu)

Degree in Progress: PhD, Physics, University of Nevada, Reno ✦ **Advisor:** Dr. Roberto C. Mancini ✦ **HEDLP:** 2014-Present

Research Topic

Laser Heating and Electron Temperature Spatial Distributions in Magnetized Plasmas Relevant to Magnetized Liner Inertial Fusion



Research Responsibilities

My research is focused on using X-ray spectroscopy to investigate the laser-heating in experiments relevant to Magnetized Liner Inertial Fusion (MagLIF). In experiments performed at the Z machine, deuterium and a trace amount of argon were placed into a cylindrical liner and heated with ~1,500 J of laser light. Two instruments were fielded to measure the X-rays emitted from the heated plasma: a spectrometer that records spatially-resolved spectra and a diagnostic that produces narrowband images of the emission. By including the spectra and narrowband image data in a multi-objective data analysis that utilizes both measurements simultaneously and self-consistently, I have extracted two-dimensional, spatial electron temperature distributions $T_e(r,z)$. With these results, I have been able to examine how inhibited thermal conduction due to an external magnetic field impacts the laser-heating, temperature distribution, and temperature gradients. I have compared these results with predictions from magneto-hydrodynamics (MHD) simulations, and I have performed a separate series of MHD simulations to investigate the role of thermal conduction during the laser heating.

Benefits of HEDLP

The HEDLP program has given me the opportunity to become involved with MagLIF and to use my research to contribute to the advancement of this fascinating approach to inertial fusion. It has allowed me to travel to meetings and conferences such as the SSAP Symposium, annual meeting of the American Physical Society (APS) Division of Plasma Physics, and the annual Omega Laser Users Group workshop. At these conferences, I have been able to present and discuss my work with experts from all across the country and receive feedback from them that has been invaluable to my research.

National Laboratory Experience

I have made several visits to Sandia National Laboratories (SNL) to discuss my work, observe experiments, and collaborate with the wonderful scientists there. I have met with SNL scientists from a wide range of backgrounds including experimentalists and theorists. This has exposed me to a variety of topics and viewpoints. I truly believe that the opportunity to meet with the scientists at SNL has had a tremendous impact on my growth as a scientist. These collaborations have introduced me to new concepts and have expanded my knowledge of my individual project and plasma physics, in general.

National Laser Users' Facility

Demonstration of Talbot-Lau X-ray Deflectometry Electron Density Diagnostic in Laser Target Interactions

Johns Hopkins University ✦ PI: Dr. Maria Pia Valdivia (mvaldiv2@jhu.edu)

X-ray refraction-based imaging diagnostics have been developed by the Johns Hopkins X-ray imaging and Plasma Spectroscopy group. Electron density diagnostics in High Energy Density Laboratory Plasmas (HEDLP) are challenging owing to small spatial and short time scales and large densities in an extreme radiation environment. Experiments have been conducted at the University of Rochester Laboratory for Laser Energetics (LLE) to benchmark a Talbot-Lau X-ray Deflectometer (TXD) for the OMEGA EP laser (EP-TXD). The diagnostic uses standard X-ray backlighters to directly measure electron density gradients and can simultaneously measure refraction, attenuation, elemental composition, and small-angle scatter.

Differential phase-contrast imaging offers a stronger contrast mechanism, since refraction signatures are much larger than attenuation when probing low-Z matter with 1-100 keV X-rays. Hence, X-ray refraction imaging techniques based on Talbot-Lau Interferometry have been developed to characterize fusion-relevant dense plasmas. Sponsored by the National Laser Users' Facility grant, the EP-TXD diagnostic platform has been established. In collaboration with researchers at the LLE and the University of Michigan, an experimental platform was designed to probe the ablation front of an irradiated foil to obtain electron density measurements above quarter critical. The experiment was designed to establish TXD by imaging, for the first time, plasma targets using laser-produced, X-ray backlighters. Electron density mapping above 10^{23} cm^{-3} will help benchmark standard magnetohydrodynamic codes which fail to accurately model ablating plasma properties. The results obtained can help validate codes with the longstanding problem of ablation dynamics in laser-produced coronal plasmas and can aid in two-plasmon decay as well as general laser-plasma interaction studies.

The EP-TXD rail is shown in Figure 1a. The G_0 grating converts the spatially incoherent backlighter into a quasi-coherent, X-ray source. The G_1 grating produces a micro-periodic fringe pattern (Talbot effect) at the location of the G_2 grating. A refracting object placed in the X-ray beam shifts this fringe pattern, producing intensity changes proportional to the refraction angle, behind G_2. This angle is proportional to the probed object electron density gradient, enabling two-dimensional electron density mapping.

A LaserNetUS experimental campaign optimized X-ray backlighter spatial resolution, emission spectra, and flux. Multi-TeraWatt preliminary experiments informed backlighter target, detector, and laser parameters for the Irradiated Foil experiment. An X-ray backlighter evaluation was performed on Omega EP, followed by ablation profile imaging. Driving beam laser parameters were adjusted in similarity to X-ray backlighter target and laser parameters. For the very first time the ablation front of an irradiated foil was imaged through TXD. A refraction angle 2D map with a measured spatial resolution of ~10 μm was obtained from the Moire deflectometry image.

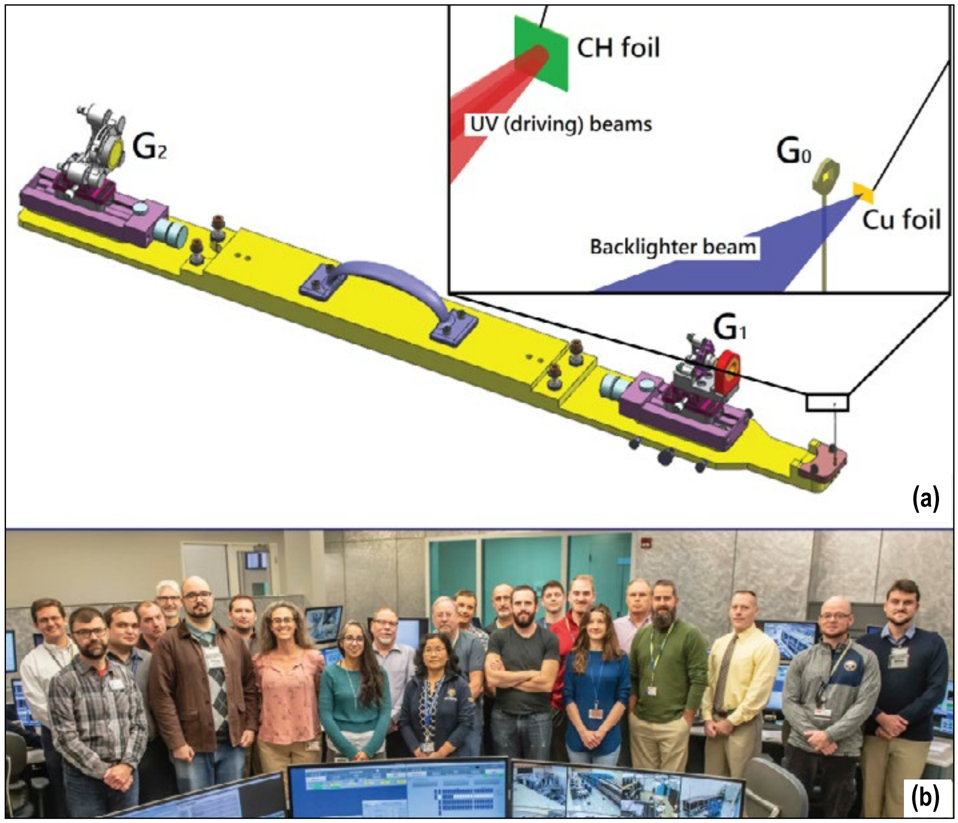


Figure 1. (a) EP-TXD diagnostic platform. b) Johns Hopkins researchers and the scientific team that participated in the FY20 EP-TXD Irradiated Foils campaign.

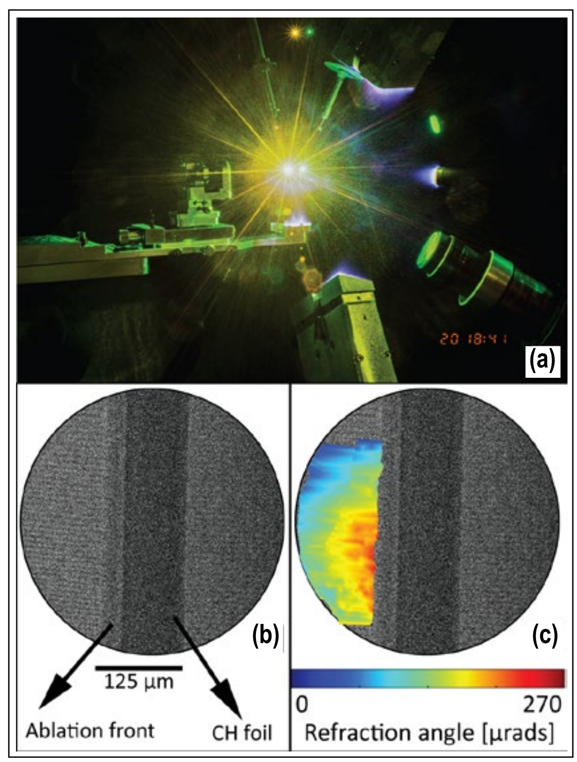


Figure 2. (a) Visible camera image of the EP-TXD diagnostic in the Irradiated Foil campaign. (b) Raw Moiré image of the 125 μm CH irradiated foil (150 J, 1 ns) obtained through TXD at 5 ns. (c) Refraction angle 2D map retrieved through TXD methods.

Colliding Megagauss Plasma Jets Experiment

Rice University ✦ PI: Dr. Edison Liang (liang@rice.edu)

An important question in the study of shock waves, in both astrophysical and laboratory plasmas, is the role of the heat flux carried by electron thermal conduction. When the electron thermal conductivity is high, the conduction front runs ahead of the shock, carries energy upstream, and lowers the post-shock electron temperature. When the electron thermal conductivity is low, the post-shock electrons and ions have roughly the same temperature. Hence, the shock structure and evolution depend strongly on the electron thermal conductivity. In magnetized shocks, the magnetic field can strongly influence the electron transport. Even if the magnetic field is dynamically unimportant ($B^2 << \rho v^2$), it still can inhibit electron thermal conductivity across field lines and influence the structure and evolution of the shock. When the electron gyroradius becomes smaller than the coulomb mean free path, thermal conduction perpendicular to the field lines becomes inhibited even when the coulomb mean free path is large while thermal conduction along the field lines remains uninhibited. In such cases electron thermal conduction can become highly anisotropic, and the structure and evolution of the shock depend strongly on the orientation and strength of the local magnetic field. Hence, our goal is to develop laboratory platforms to systematically study strongly magnetized shocks in controllable settings.

In a series of OMEGA laser experiments in 2016 and 2017,[1,2] we demonstrated that a hollow ring configuration of 20 OMEGA beams irradiating a flat disk can create narrowly collimated megagauss (MG) plasma jets. In such strongly magnetized jets the electron gyroradii can become much smaller than the coulomb mean free path. Hence, we expect that electron thermal conduction will become highly anisotropic. When two such jets collide head on, they will create strongly magnetized, high-beta shocks which should provide a unique platform to study the effects of anisotropic electron thermal conduction on shock structure and evolution. Subsequent three-dimensional (3D) FLASH simulations show that the collision of two MG plasma jets, each created by 20 OMEGA beams in a hollow ring pattern, will indeed launch two expanding shocks whose structure and evolution strongly depend on the local magnetic field geometry and electron thermal conductivity. We were awarded one OMEGA shot date in 2020 and one joint shot date in 2021 to carry out such colliding jets experiments. At the writing of this report, we just completed our 2020 experiment, but the data have not yet been analyzed. However, preliminary X-Ray Framing Camera (XRFC) images show that expanding shocks indeed were created. We are cautiously optimistic that the data from our 2020 colliding jets experimental will shed new light on this important question.

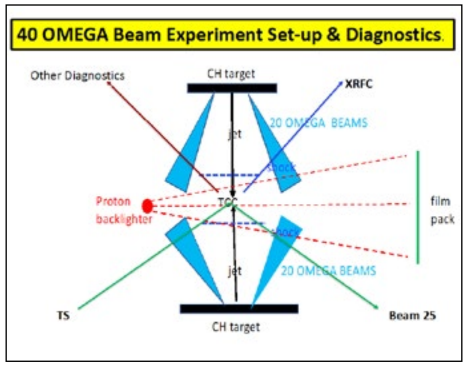
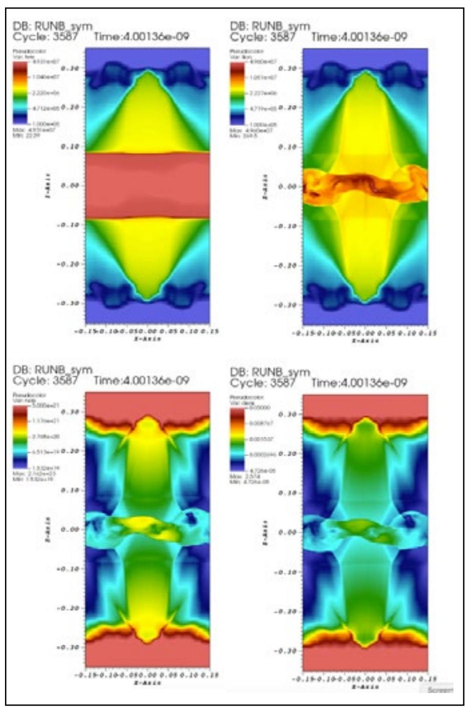


Figure 1. Sketch of experimental setup of colliding MG jets experiment using 40 OMEGA beams.

Figure1 is a sketch of the colliding jets experimental setup. 20 OMEGA beams from each hemisphere irradiate a flat CH target with a hollow ring pattern of radius = 800 microns and target separation = 6.4 mm. The Thomson Scattering diagnostic is used to measure the density, electron and ion temperatures, and flow velocity at the Target Chamber Center (TCC) and 150 microns below the TCC. Protons from a D^3He fusion capsule are used to map out the magnetic field geometry and amplitude. In addition, an XRFC is used to capture time-lapse, X-ray images of the entire domain. Figure 2 shows 3D FLASH simulation results of this experiment at 4 ns, based on Spitzer thermal conductivity, plus lineout plots along the jet axis. Both the expanding electron conduction fronts and shock fronts are visible with the conduction front running ahead of the shocks. These predictions will be confronted with our 2020 experimental data. We anticipate the analyses of our 2020 data to be completed in early 2021. This will give us ample time to finalize and refine the design of the follow-on experiment with more advanced diagnostics that currently is scheduled for August 2021.



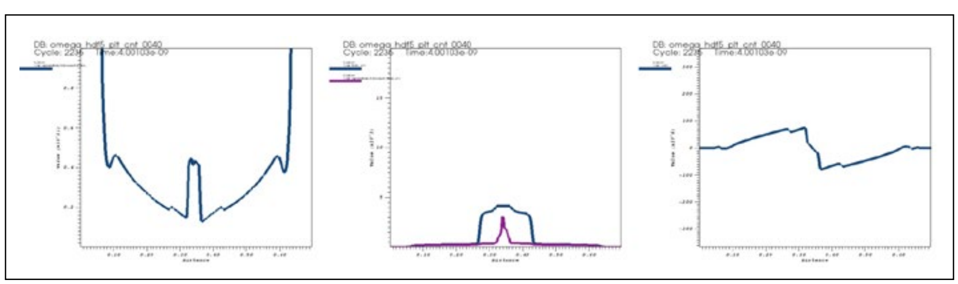


Figure 2. Color figures: 3D FLASH- simulated profiles of shocked electron temperature (top left), ion temperature (top right), electron density (lower left), and ion density (lower right) at 4 ns. Line plots: Profiles along the jet axis of (left) density, (middle) electron (blue), and ion (purple) temperatures, and (right) axial velocity at 4 ns.

References

[1]L. Gao et al., 2019, ApJL, 873, L11.

[2]Y. Lu et al., 2019, PoP 26, 022902.

"...effective interactions with experimentalists at Omega and Lawrence Livermore National Laboratory helped us to interpret the myriad diagnostic details correctly and to extract 3D temperature and density maps of an ICF plasma for the first time. Presentation of this research at multiple major conferences, with the support of the NLUF grant, helped to maximize my career opportunities."

— Dr. Taisuke Nagayama
Sandia National Laboratories

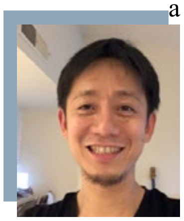
"The NLUF program has helped me through my PhD tremendously, and it has given me the opportunity to meet with several experts in my field."

— Dylan Cliche
University of Nevada, Reno

"At LANL, I was provided with invaluable opportunities to work with scientists of various computational and experimental disciplines."

— Yingchao Lu
Rice University

Taisuke Nagayama, Sandia National Laboratories (tnnagay@sandia.gov)
Years at SNL: September 2011-Present ✦ **Degree:** PhD, Physics ✦ **NLUF Program:** 2006-2011, University of Nevada, Reno



I am a staff scientist at Sandia National Laboratories (SNL) engaged in multiple, fundamental science projects and leading the modeling and data analysis of stellar opacity experiments. Our experiments on the Z pulsed power facility have raised questions about opacity, the property that controls energy transport in stars and materials. That research was published in Nature, because of its critical implications to other applications and resulted in our team receiving an NNSA Defense Program Award of Excellence in 2015. I am collaborating with theorists to improve the predictability of material property simulations, which is of importance to national security. I have found that research at SNL is collegial and full of learning via interactions with some of the world's finest experimentalists and theorists. When I started my PhD program at University of Nevada Reno, my dream was to work at a national laboratory. Today, I collaborate with top scientists to solve mission-critical problems. The National Laser Users Facility (NLUF) played a vital role in my learning and in my seamless transition to SNL.

When I started my PhD program under Professor Roberto C. Mancini, I was unsure what path my career might take. The focus of Roberto's group was on diagnosing the temperature and density spatial profiles of inertial confinement fusion (ICF) plasmas using multi-monochromatic imagers (MMIs) (Figure 1). Such diagnostics are desirable to understand what happens in ICF experiments. An MMI records spectra with two-dimensional spatial resolution. My goal was to develop a tool to analyze the MMI data and to extract three-dimensional (3D) temperature and density maps of an ICF plasma. Whereas this project involved extensive coding and testing, the programming aspect was a relatively minor challenge thanks to my computer science education. The bigger challenges were 1) understanding ICF and how X-rays are generated through atomic processes in plasmas (APiP) and 2) obtaining high-quality MMI data and properly interpreting the meaning of each pixel of data. I learned that advancing the state-of-the-art in science involves more than one can absorb from journal articles and conference presentations.

> *"Today, I am honored with invitations to speak at major conferences, asked to review high-impact journal articles, and help with organizing APiP and ICF conferences. The opportunities and training through NLUF and the Academic Programs made this challenging and fun journey possible."*

For more practical learning, I simplified my strategy: 1) breaking down my questions, 2) finding a mentor who is knowledgeable and honest about his or her understanding, and 3) asking him or her questions. This question-driven learning worked extremely well. My understanding about APiP and ICF improved dramatically through persistent questioning together with suggested readings. Back then, I thought I made this expanded learning happen. Now I realize I was taking advantage of the institutionalized knowledge of all my mentors who were trained and/or funded by NLUF and the Academic Programs.

High quality data and excellent support from the Omega Laser Facility operated for NLUF made the first 3D temperature and density analysis possible. Omega allowed us to obtain high quality MMI data. At the same time, effective interactions with experimentalists at Omega and Lawrence Livermore National Laboratory (LLNL) helped us to interpret the myriad diagnostic details correctly and to extract 3D temperature and density maps of an ICF plasma for the first time. Presentation of this research at multiple major conferences, with the support of the NLUF grant, helped to maximize my career opportunities. I received three postdoctoral fellowship offers and chose SNL to expand my scientific vision and to get high visibility to become a staff scientist. I accomplished both goals in three years.

Today, I am honored with invitations to speak at major conferences, asked to review high-impact journal articles, and help with organizing APiP and ICF conferences. The opportunities and training through NLUF and the Academic Programs made this challenging and fun journey possible.

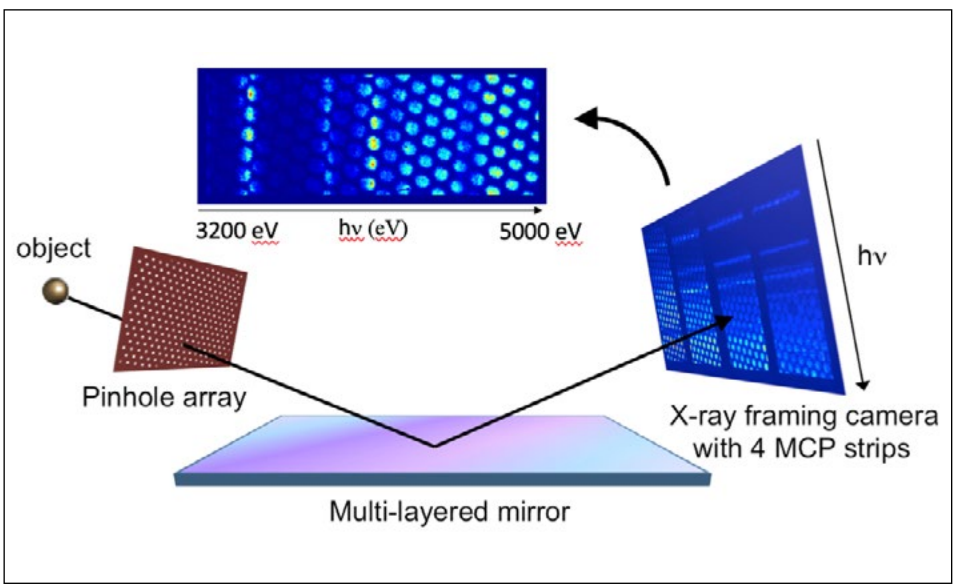
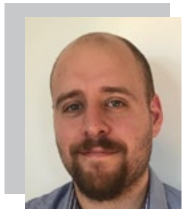


Figure 1. A multi-monochromatic imager, MMI, consists of a pinhole-array, multi-layered mirror, and microchannel plate (MCP), which records hundreds of object images with a horizontal photon-energy axis.

Dylan Cliche (dcliche@gmail.edu)

Degree: PhD, Physics, University of Nevada, Reno (December 2020) ✦ **Advisor:** Dr. Roberto C. Mancini ✦ **NLUF:** 2017-Present



Research Topic

Understanding and Furthering the Applications of X-ray Multi-Monochromatic Imaging with the Multi-Monochromatic X-Ray Imager Instrument

Research Responsibilities

Half of my research involves deepening our understanding of the multi-monochromatic X-ray imager (MMI) instrument. The MMI is an instrument comprised of a pinhole array coupled to a multi-layered Bragg mirror to record an array of spectrally resolved, two-dimensional images of inertial confinement fusion (ICF) plasmas on a time-gated microchannel plate-based detector. The characteristics of the instrument previously were derived in a parallax ray approximation. I introduced an advanced model to better understand the instrument by writing a three-dimensional X-ray tracing code that can better characterize the MMI and produce higher fidelity synthetic MMI data.

The other half of my research furthers the applications of the MMI. The MMI originally was designed to record X-ray line spectra from spectroscopic tracers to extract the electron temperature and density spatial profiles in the ICF plasma. For the first time, we recently were able to record arrays of images based on continuum emission to extract electron temperature and compressed-shell optical depth maps. This opens the door to using the MMI on dopant-free, ignition-type ICF implosions to study their asymmetries and correlation with implosion hydrodynamics. We have utilized the ability to extract spatially-resolved spectra from MMI data to obtain spatial profiles of the electron temperature and density as well as to establish a novel analysis to extract the mixing between fuel and shell material that relies on the radiation transport effect on Stark-broadened spectral line shapes.

Benefits of NLUF

The NLUF program has helped me through my PhD tremendously, and it has given me the opportunity to meet with several experts in my field. The ability to speak with people in all the programs sponsored by the Academic Programs has helped to broaden my horizon and gives me new and broader insights into my work. This has led to bettering my research as well as future employment opportunities.

National Laboratory Experience

I traveled to Los Alamos National Laboratory each summer from 2014 to 2019. During this time, I learned how to run their xRAGE code to simulate ICF experiments from our National Laser Users' Facility campaigns. This helped me to determine what physics were the largest contributions to what we were seeing experimentally. Along with learning the xRAGE code, I was able to learn about hydrodynamics, plasma physics, and mixing models from some of the world's leading experts.

Yingchao Lu (yingchao.lu@gmail.com)

Degree in Progress: PhD, Physics, Rice University ✦ **Advisor:** Dr. Edison Liang ✦ **NLUF:** 2016-Present

Research Topic

Magnetic Fields in High Energy Density, Laser-Driven Plasmas

Research Responsibilities

As a graduate research assistant in the Department of Physics and Astronomy at Rice University and in the Theoretical Division at Los Alamos National Laboratory (LANL), my primary research responsibility is to carry out radiation-magnetohydrodynamics simulations using the FLASH code to model high energy density (HED), laser-driven plasmas and to study the role of magnetic fields in these plasmas. I have been working on two experimental platforms on the OMEGA laser facility. One is on the magnetized jet driven by a hollow ring of laser beams lead by Rice University and the Princeton Plasma Physics Laboratory. The second is on the magnetic field generation in shock-shear targets lead by the team at LANL. In order to quantitatively understand the data from these experiments, I have used codes to generate the synthetic X-ray images, Thomson scattering spectra, and proton images. Because of the high-density condition in the shock-shear targets, I wrote a Monte Carlo code, MPRAD, that uses the results of FLASH simulation as input and takes into account the stopping power and Coulomb scattering of the proton beam in the Monte Carlo modeling.

Benefits of NLUF

The magnetized jet experiments and simulations that I have been working on are supported by the National Laser Users' Facility program. I attended the annual Stewardship Science Academic Programs symposium and OMEGA Laser User Group workshop where I met researchers from other universities and institutions and learned about frontier research in HED science. Being a part of the NLUF program has allowed me to collaborate with scientists at LANL and has accelerated my progress in the graduate program.

National Laboratory Experience

I spent two and half years at LANL as a graduate research assistant. The research environment at LANL is quite different from my home graduate school. At LANL, I was provided with invaluable opportunities to work with scientists of various computational and experimental disciplines. The discussion with the experimental scientists has helped me to better understand how to use simulations to optimize the OMEGA experiments. The computational resources and the help from experts on numerical simulations at LANL accelerated my research progress on a few computational projects. I believe that my experience at LANL will be beneficial to my research in the future even beyond my graduate program.

Predictive Science Academic Alliance Program III

Center for Hybrid Rocket Exascale Simulation Technology

University of Buffalo ✦ PI: Dr. Paul DesJardin (ped3@buffalo.edu)

The Center for Hybrid Rocket Exascale Simulation Technology (CHREST) was founded in the fall of 2020. CHREST aims to advance space exploration through interdisciplinary research that will improve the operation of hybrid rocket motors and enable the next generation of low-cost space flight.

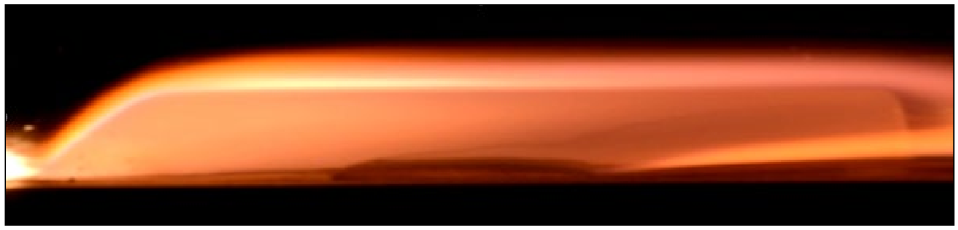


Figure 1. Slab motor experiment showing the burning of paraffin wax fuel used in hybrid rockets.

The Problem

Low-cost access to space has never been in higher demand, and launch costs are driven principally by the propulsion system. Existing liquid propulsion systems are complex and seem to have reached the limit for fuel energy density. A breakthrough on propellant that significantly increases the energy density, or specific impulse, of the propellant would greatly reduce launch costs, accelerating access to space and its industrial development.

Practical operation of high-regression rate, hybrid rocket motors is of great interest, because they can provide the sought-after blend of the high energy density of solid bi-propellant systems with the specific impulse and flexibility of liquid-fueled, air-breathing engines. These fuels burn differently from traditional polymeric fuels in that they form a thin liquefaction layer at the solid fuel surface where instability leads to atomization and enhanced burning rates (Figure 1). Practical hybrid motors, however, have not yet been realized due to limited understanding and control of precise combustion burning modes and thermo-mechanical coupling at the interface.

Technical Challenge

A hybrid rocket motor works by combining a segregated solid fuel with a gaseous oxidizer, e.g., air or liquid oxygen (LOX). The challenge of operating a hybrid rocket motor is controlling the turbulent flow physics at the fuel-oxidizer interface which is dominated by conjugate heat and mass transfer and combustion processes.

The focus of the newly formed CHREST is to leverage advances in both exascale computing and machine learning to better understand the turbulent, multiphase mixing, and fuel entrainment in the combustion environment that is so critical to the operation of these systems.

CHREST will bring together faculty and students from the University at Buffalo (UB) and Tufts University who specialize in engineering, computer science, and mathematics, to combine new mathematical models with first-principles' simulation of hybrid rocket motors to enable a next-generation of low-cost space flight.

The Center will utilize extremely powerful computers to simulate previously developed hybrid rockets as well as future theoretical rockets. The team also will develop machine learning algorithms that offer insight into how to better design hybrid rockets.

Educational Component

CHREST is establishing a vibrant program to educate UB students about hybrid technology. The Center will support UB's Students for the Exploration and Development of Space (SEDS), an undergraduate student club that designs, builds, tests and launches rockets (Figure 2). The club competes in the annual Spaceport America Cup, the world's largest intercollegiate rocket engineering conference and competition.

The program aims to recruit students from groups underrepresented in science, technology, engineering, and math fields. This includes working with established programs such as the Louis Stokes Alliance for Minority Participation, more commonly known as LSAMP, and Buffalo-area Engineering Awareness for Minorities, also known as BEAM, to provide students with hands-on research experiences in a developing field.

Outcomes

Potential future uses of hybrid rockets include launching satellites, especially nanosatellites, into space from Earth. Such systems also could be very useful

CHREST
Center for Hybrid Rocket Exascale Simulation Technology

Figure 2. CHREST will support SEDS, a UB student club that builds rockets.

in situations where high thrust is required to lift heavy payloads loads into space from planetary surfaces, such as NASA's planned Mars Ascent mission.

Funding

The Center is supported through the recently announced third generation Predictive Science Academic Alliance Program of the Department of Energy/ National Nuclear Security Administration.

For more information, visit https://buffalo.edu/chrest.

Micromorphic Multiphysics Porous and Particulate Materials Simulations within Exascale Computing Workflows

University of Colorado Boulder ✦ PI: Dr. Richard Regueiro (richard.regueiro@colorado.edu)

The overall objective of the Multi-disciplinary Simulation Center (MSC) is to simulate with quantified uncertainty, from pore-particle-to-continuum-scales, a class of problems involving granular flows, large deformations, and fracture/fragmentation of unbonded and bonded particulate materials. The overarching problem is the processing and thermo-mechanical behavior of compressed virgin and recycled mock high explosive (HE) material subjected to quasi-static and high- strain-rate, confined and unconfined compression, in-situ quasi-static X-ray computed tomography, and dynamic (impact) experiments with ultrafast synchrotron X-ray imaging at the Advanced Photon Source (APS) at Argonne National Laboratory.

To accomplish the objective, a micromorphic, multiphysics, multiscale computational framework will be developed, verified, and validated with quantified uncertainty and executed on exascale computing platforms seamlessly through a scientific software workflow to reduce the full-time-equivalent effort on handling data from the beginning to the end of simulation. Machine Learning (ML) algorithms will be applied to fill the gaps in multiscale, constitutive modeling via coordinated pore-particle-scale experiments and Direct Numerical Simulations (DNS). Integrated experimental testing at quasi-static and dynamic rates (including ultrafast synchrotron x-ray imaging at the APS and proton imaging at Los Alamos National Laboratory's pRad facility) at length scales ranging from pore-particle to continuum scales will be conducted to validate heterogeneous, pore-particle-to-continuum-scale, computational models, calibrate model parameters, and validate the overall computational framework. Exascale computing is needed to simulate these more sophisticated micromorphic, multiphysics, bridged-DNS simulations, with offline ML training of micromorphic constitutive relations to DNS. Furthermore, for validation and uncertainty quantification (UQ) requiring multiple instances of these simulations over statistical distributions of inputs (such as particle size distribution), with high and low fidelity, Exascale computing is a necessity.

The MSC research will usher in a new era of higher-fidelity, multiscale, multiphysics computation through large deformation, micromorphic, continuum field theories informed by DNS through the latest ML techniques calibrated and validated against a rich experimental data set. Applying advances in verification and validation (V&V)/UQ, Exascale computing and Integration/Workflows will make the applicability of such an approach to reduce uncertainty in continuum-scale computations based on statistical distributions of materials' information at the pore-particle-scale of bonded particulate materials a reality, which has significant influence on the success of the Stockpile Stewardship Program for HE materials and beyond.

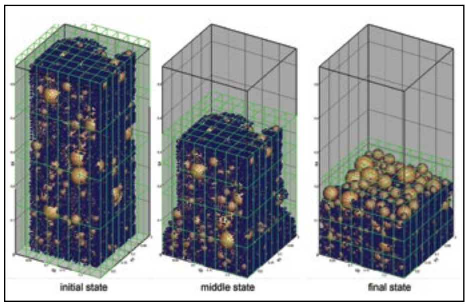


Figure 1. Simulation of particle gravity deposition with hybrid OpenMP-MPI Discrete Element Method (DEM) code ParaEllip3d. Maximum to minimum particle diameter ratio = 10.

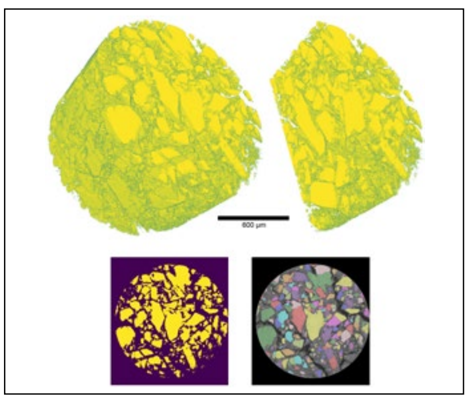


Figure 2. Computed Tomography (CT) image (top) of mock HE, courtesy of B.M. Patterson and J.D. Yeager (LANL), with watershed segmentation (bottom) by C.G. Becker and A.J. Clarke (Colorado School of Mines).

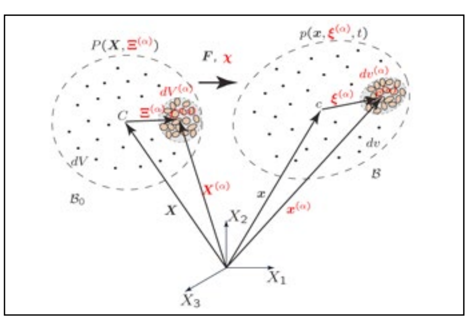


Figure 3. Illustration of mapping from reference to current configurations in micromorphic continuum field theories.

Micromorphic continuum field theories are the most general type of generalized continuum field theory, described by Kröner (1968)[1] as "bridging of the gap between microscopic (or atomic) research on mechanics on one hand, and the phenomenological (or continuum mechanical) approach on the other hand," and by Green and Naghdi (1995)[2] as a "body embedded in a ... three-dimensional space with each of its material points endowed with additional kinematic structure." Eringen (1999)[3] stated that, "The concept of microcontinuum naturally brings length and time scales into field theories. The response of the body is influenced heavily with the ratio of the characteristic length λ (associated with the external stimuli) to the internal characteristic length ℓ. When λ/ℓ » 1, the classical field theories give reliable predictions since, in this case, a large number of particles act collaboratively. However, when λ/ℓ ≈ 1, the response of constituent subcontinua (particles) becomes important, so that the axiom of locality underlying classical field theories fails."

MSC activities for FY 2021 include: (1) uploading and managing all source code on gitlab.com/micromorph; (2) recruiting US citizen, graduate students; (3) obtaining materials (glass beads, aluminum spheres and shot, silica sand, idoxuridine (IDOX) crystals, and Estane binder) to begin experiments and perform initial computed tomography of model particle/matrix composites at the APS (mail-in beam time) to inform computational efforts; (4) establish V&V/UQ simulation and experimental workflow on gitlab.com/micromorph/share; and (5) begin design and development of extension to heterogeneous central processing unit/graphics processing unit simulation for ParaEllip3d-CFD (DNS DEM-MPM-CFD) and Tardigrade (micromorphic continuum with upscaling) codes.

Visit micromorph.gitlab.io to learn more.

References

[1]E. Kröner, Ed. Mechanics of Generalized Continua. Springer-Verlag, 1968.

[2]A.E. Green and P.M. Naghdi. Unified procedure for construction of theories of deformable media. II. Generalized continua. Proc. R. Soc. Lond. A, Math. Phys. Eng. Sci., 448(1934):357-377, 1995.

[3]A.C. Eringen. Microcontinuum Field Theories I: Foundations and Solids. Springer-Verlag, 1999.

Center for Exascale-enabled Scramjet Design

University of Illinois at Urbana-Champaign ✦ PI: Dr. Jonathan Freund (jbfreund@illinois.edu); Co-Director: Dr. William Gropp

The new Center for Exascale-enabled Scramjet Design seeks to use predictive science simulations, enabled by the efficient use of massive-scale computational resources, to advance scramjet design through the use of lightweight, high-temperature, composite materials. The center is designed to meet predictive science objectives and, at the same time, to provide a rich context for in-depth PhD studies of high-risk opportunities for advancing computational science.

A scramjet—a supersonic combustion ram jet—is an air-breathing, propulsion system capable of operating at extremely high speeds, well above the nominal hypersonics threshold of Mach 5. Because it is air-breathing, it avoids the weight penalty of a rocket's onboard oxidizer, which makes it attractive for access to space and for next-generation delivery systems. However, the extreme condition of such a device presents significant challenges for engineering design. High-temperature, composite materials offer a rich design space, enabling greater robustness, improved performance, and flexibility across the flight envelope. This center will consider multiple strategies for their use: dense and strong heat-resistant composites, flexible composites for shape morphing, and composites designed for thermal protection by ablation, similar to some atmospheric entry systems. The extreme conditions make experimental testing a challenge. Flight tests are expensive, as are at-scale ground tests, and diagnostics are extremely limited for both.

Physics-based, predictive simulations will offer a unique opportunity to evaluate design concepts and optimize them while being cognizant of the underlying physics. This, however, will require the integration of many physical sub-mechanisms: compressible flow dynamics, turbulent mixing, chemical combustion, and the interaction of the high-temperature, combusting mixtures with composites comprised of complex microstructures. The degradation of these depend on complex, surface-oxidation processes and how they interact with the thermochemical environment within the microstructure of the materials. Important scales span from that of the engine down to micron-scale, carbon fiber features, and behavior depends on the fast time scales of turbulent mixing and surface chemistry to the slow cumulative effects of oxidation and fracture. Figure 1 shows a demonstration of a degrading carbon fiber matrix, in this case unprotected by any coating, in a short test firing of the Arc Heated Combustion Tunnel-II (ACT-II) facility on the Illinois campus. This facility will provide our primary prediction target.

Several physical components of the system, such as turbulent combustion and thermal conduction in the microstructural materials, are such that predictive confidence can be secured through the resolution of length and time scales. Yet to do this demands massive-scale computation, directly benefiting from the efficient utilization of high-performance computing resources. To achieve this, as we move along the path to exascale computing and beyond, will require meeting two opposed challenges: keeping code hardware flexible to adapt to evolving architectures while maintaining usability and adaptability by the computational scientists who develop and run them. The primary computer science research of the center is a path for meeting these dual objectives. An intermediate representation (using Loopy) will provide sufficient abstractions for flexible kernel fusions and other operations to facilitate multi-hardware efficiency via standard code-generation tools (e.g., for OpenCL). It will provide some not-too-onerous constraints on low-level (but human readable) computational kernels, which are invoked to discretize a high-level expression of the physics in user-friendly Python. This MIRGE (Math—Intermediate Representation—Generation—Execution) framework will be used to develop a discontinuous Galerkin turbulent combustion solver (MIRGE-Com) for predictions, which will couple directly with detailed physical models for the (possibly degrading) composite walls of the combustor. Figure 2 is a schematic of the end-to-end MIRGE framework.

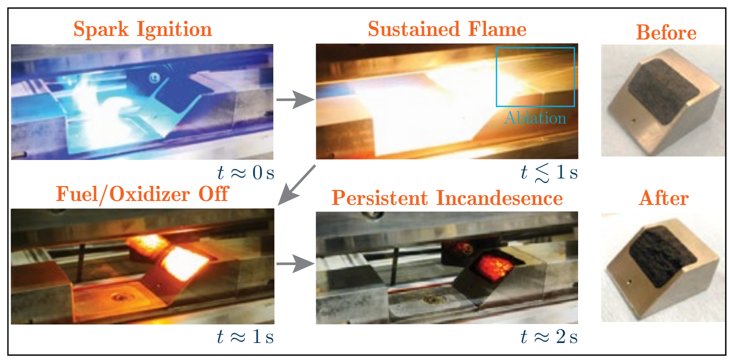


Figure 1. Mach 2.7 supersonic combustion with carbon fiber insert: an example prediction target in the Illinois ACT-II arc-driven supersonic combustion tunnel (designed and operated by CEESD co-PI Tonghun Lee with Air Force Office of Scientific Research AFOSR funding). There is obvious degradation of the model carbon fiber composite, here a surrogate for more practical engineering materials.

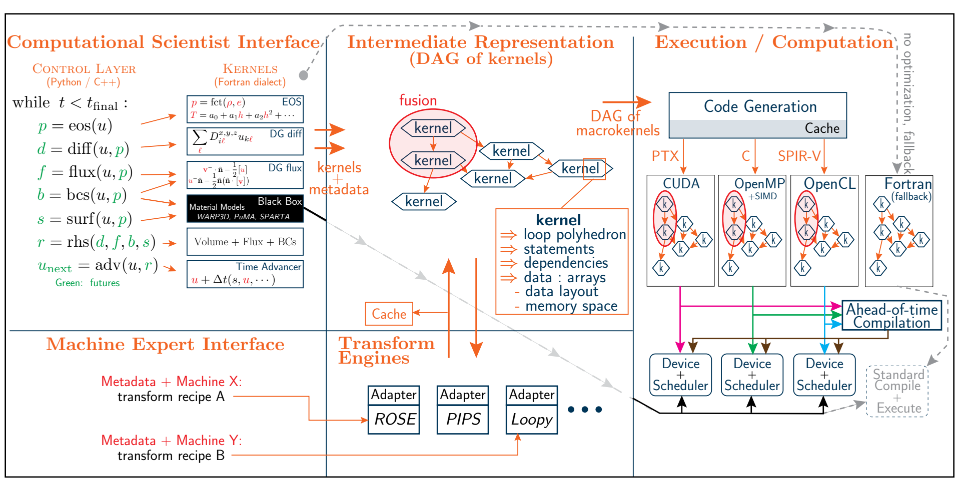


Figure 2. The MIRGE computer science framework, designed to balance usability (with python-based control layer) against portability, which is facilitated by the abstractions of the intermediate representation and existing hardware-targeted code-generation tools.

Center for the Exascale Simulation of Material Interfaces in Extreme Environments

Massachusetts Institute of Technology ✦ PI: Dr. Youssef Marzouk (ymarz@mit.edu)

The Center for Exascale Simulation of Materials in Extreme Environments (CESMIX) is a new, single-discipline center supported by the DOE/NNSA PSAAP III program located at the Massachusetts Institute of Technology (MIT).

CESMIX seeks to advance the state-of-the-art in predictive simulation by connecting quantum and molecular simulations of materials with state-of-the-art programming languages, compiler technologies, and software performance engineering tools underpinned by rigorous approaches to statistical inference and uncertainty quantification.

Our overarching goal is to predict from first principles the degradation of complex materials in extreme environments. As an exemplar of this goal, we consider hypersonics. Our aim is to simulate materials exposed to ultra-high temperatures, extreme heat fluxes, and oxidative chemical environments as on the leading edges of hypersonic vehicles (Figure 1). This setting generally is inaccessible to direct experimental observation. Significant research has been devoted to the development of better protective materials for hypersonic flight. Diborides such as HfB_2 and ZrB_2 are attractive due to their high melting temperatures, but their oxidation resistance is not ideal. High-entropy alloys of diborides promise to combine temperature and oxidation resistance with mechanical strength. But predicting these material properties is enormously difficult. Indeed, high-entropy ceramics and glassy materials with complex interfaces and oxidative processes present major challenges to available methodology. We will address these challenges by developing a comprehensive new multiscale materials simulation framework, bridging from multiple levels of electronic structure theory to hybrid quantum/classical methods (Figure 2) to classical molecular dynamics.

To generate realistic loading conditions for our materials, we will consider the aerothermal environment produced by a hypersonic shock-shock interaction around a circular cylinder. This hypersonic flow is representative of conditions at scramjet leading edges, is highly sensitive to the configuration of the shock structures, and can induce extreme and localized

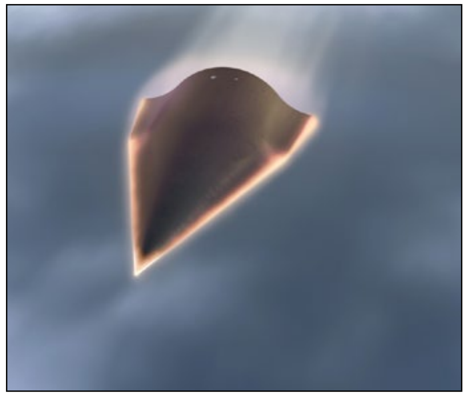


Figure 1. Illustration of a hypersonic glide vehicle, the Hypersonic Technology Vehicle 2, developed as part of the Defense Advanced Research Projects Agency (DARPA) Falcon project. (Image credit: DARPA).

surface heating. In these situations, material damage starts at the surface and propagates into the bulk. Interfaces then are crucial to our ability to understand, engineer, and control material behavior. Predictive simulation of these interfaces—their properties, evolution, and impact—is our core challenge.

Tackling this predictive simulation problem will drive the development of new exascale computing capabilities in the broadest sense: compiler technologies aimed at both portability and composable performance on heterogeneous architectures; high-level and domain-specific languages; semantic augmentation to enable differentiable programming with both new and legacy codebases; and new toolchains that facilitate uncertainty quantification (UQ) and inference across scales. Our UQ effort will support an automated "decision engine" that determines how to optimally deploy and combine models to reach a targeted uncertainty in a system-level prediction. Our simulations and UQ efforts will be supported by a unique, in-house source of high-temperature validation data.

In bringing these objectives to fruition, we expect to collaborate closely with the National Nuclear Security Administration laboratories. We will broadly disseminate our results via conferences and open-source software, and we will use our efforts to shape new interdisciplinary computational science and computer science graduate education programs at MIT.

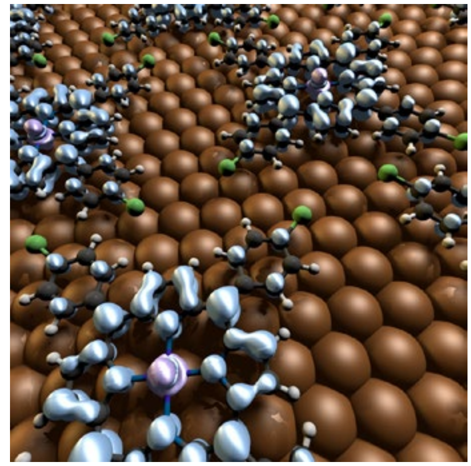


Figure 2. Density functional theory simulations of surface chemical interactions. (Image credit: H.J. Kulik, MIT).

CESMIX participants include eight faculty co-PIs spanning five MIT departments, the MIT Center for Computational Science and Engineering, and the MIT Computer Science and Artificial Intelligence Laboratory: Saman Amarasinghe, Alan Edelman, Nicolas Hadjiconstantinou, Asegun Henry, Heather Kulik, Charles Leiserson, Youssef Marzouk (PI), and Jaime Peraire. We currently are building up the rest of the CESMIX team with several research scientists, postdoctoral fellows, and students already on board along with a chief software architect, Cuong Nguyen. In steady-state, the project will support roughly three postdoctoral fellows, seven graduate students, two research scientists, and the chief software architect.

Center for Exascale Monte Carlo Neutron Transport

Oregon State University ✦ PI: Dr. Todd Palmer (todd.palmer@oregonstate.edu)

Figure 1. Members of the CEMeNT Team.

The random quantum processes that govern neutron transport lead to a variety of phenomena important to stockpile stewardship. At the Center for Exascale Monte Carlo Neutron Transport (CEMeNT), we have assembled, via a process with a smaller degree of stochasticity, three university partners (Oregon State University, North Carolina State University, and the University of Notre Dame) to create a Focused Investigatory Center (FIC) with the mission to create an advanced, dynamic, exascale Monte Carlo neutron transport simulation capability. The history of predictive science modeling and simulation at the National Nuclear Security Administration (NNSA) laboratories and as a branch of science is tied to Monte Carlo neutron (and other particle) transport. Dynamic Monte Carlo neutron transport is an essential element of many multiphysics simulations that occur at the NNSA laboratories, and we intend to assess high-risk/high-reward approaches to the solution of this single-physics problem in the context of their promise for application to coupled, multiphysics simulations. We believe our research will directly impact the programs in dynamic Monte Carlo simulation supported by the NNSA.

The team involves four prominent members of the computational nuclear science and engineering community with direct experience developing novel radiation transport algorithms, creating and testing software, and using sophisticated multi-physics modeling and simulation tools (Figure 1). In addition, CEMeNT includes experts in applied mathematics, exascale software engineering, graphics processing unit/central processing unit (GPU/CPU) hardware, and computer science in heterogeneous computing systems to create the critical mass necessary for this interdisciplinary effort.

CEMeNT's activities are collaborative and include research and development, production/testing and sharing of open-source software, education and mentoring of graduate students and postdoctoral researchers, outreach to and recruitment of traditionally underrepresented minority populations, and peer-review and dissemination of scientific results.

The software engineering thrust of CEMeNT will focus on enabling the solution of Monte Carlo neutron transport problems on anticipated exascale platforms involving heterogeneous computing devices. Our team involves three experts in optimization of algorithms and software development for heterogeneous devices with CPUs and GPUs. Many of our team members have experience in high-performance computing and are adept in multiphysics modeling and simulation on large-scale parallel machines.

Specific, novel, technical advances associated with CEMeNT will include: the capability to perform dynamic Monte Carlo neutron transport simulations (including a census of particles), built-in uncertainty quantification for stochastic solution techniques, advanced code and solution verification techniques for stochastic simulation, machine-learning-based optimization of parameters in large, heterogeneous, high-performance computing, investigation of a multi-level, hybrid, deterministic/Monte Carlo approach for improved efficiency and variance reduction, and development of domain decomposition techniques for the enhancement of parallel computation performance. Additionally, modern software and techniques for nuclear data processing will be heavily utilized by the team. The effort of integrating computational and experimental results will be performed by members of our team with a history of running multiphysics nuclear weapons codes, Monte Carlo neutron transport tools, and visualization and data mining in large data sets.

CEMeNT will have agile and inclusive management practices, be tightly connected to researchers at the NNSA national laboratories, and will leverage existing research relationships and computing facilities to amplify the existing and previous successes of the individual participating faculty researchers in advancing the field and training future NNSA laboratory staff members.

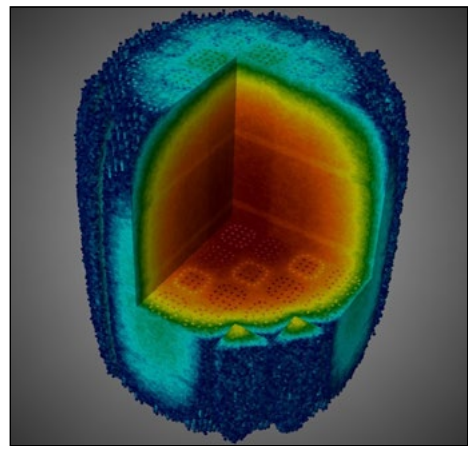


Figure 2. Small modular reactor neutron flux contours from Shift.

In the inaugural year of our FIC, we will develop direct experience performing steady-state and eigenvalue simulations with Oak Ridge National Laboratory's Shift Monte Carlo particle transport code and develop our strategy for integrating census to implement time-stepping. Year 1 entails designing the structure and composition of the Python-based, Monte Carlo platform for experimenting with new algorithms and code generation tools for parallelizing on distributed memory systems.

Integrated Simulations Using Exascale Multiphysics Ensembles

Stanford University ✦ PI: Dr. Gianluca Iaccarino (jops@stanford.edu); Author: Javier Urzay and Gianluca Iaccarino

The overarching problem of the Integrated Simulations using Exascale Multiphysics Ensembles (INSIEME) project is the prediction of reliability of in-space ignition of cryogenic propellants (gaseous methane and liquid oxygen) in a model rocket combustor (Figure 1). The problem involves a broad set of physical phenomena, such as multiphase, compressible, fluid dynamics, thermodynamics, turbulent mixing, laser-induced ignition, and combustion. In the initial stage at near-vacuum pressures, the rocket combustion chamber is primed with one of the propellants. Once the pressure has reached a sufficiently high value suitable for chemical reactions to occur, a non-resonant laser triggers ignition of the cryogenic propellants and gives rise to a secondary stage that includes flame propagation and stabilization in the combustor. The whole process of ignition is very fast but is nonetheless crucial for the success of flight missions in real space engineering applications.

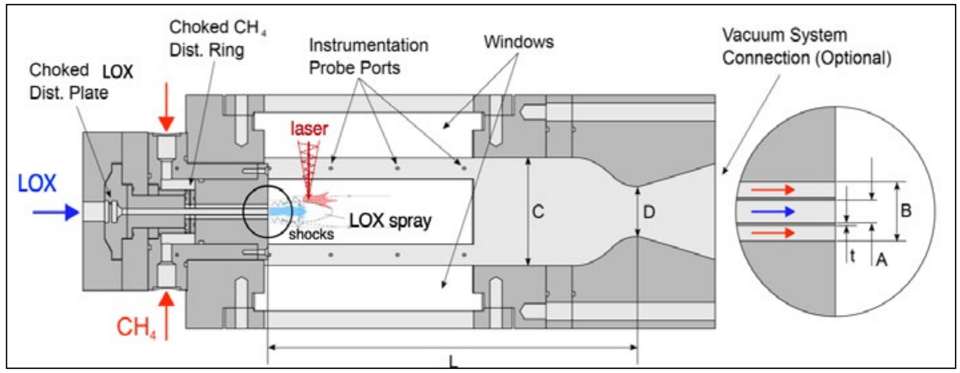


Figure 1. Computer-aided design schematics of the INSIEME experimental rocket-combustor geometry (courtesy of Carson Slabaugh, Purdue University).

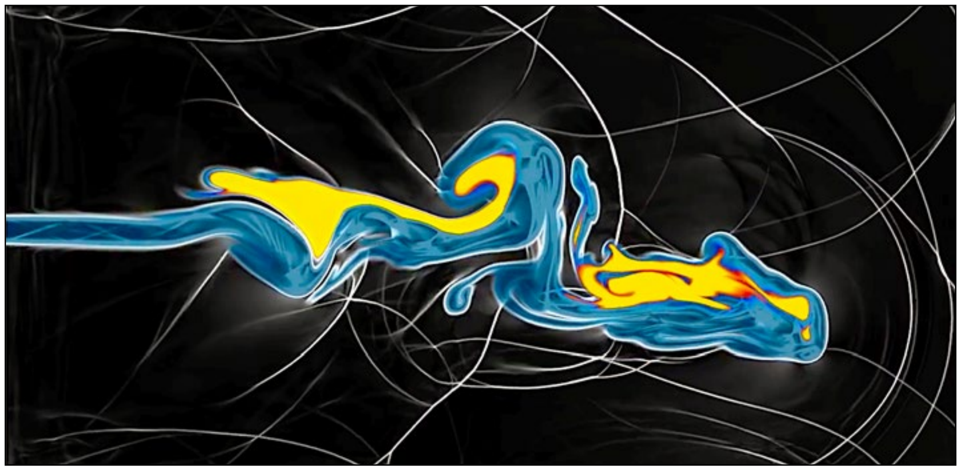


Figure 2. Preliminary simulations of laser-induced ignition using the Center's task-based simulation software (Courtesy of Dr. Mario Di Renzo and Dr. Kazuki Maeda).

Achieving ignition in a rocket combustor using lasers relies on the appropriate timing and location of the laser energy deposition. Important quantities influencing the ignition process that make it highly stochastic in practical combustor flow environments are the local temperature, equivalence ratio, and turbulent intensities. These quantities are sensitive to aerodynamic effects induced by shock waves, turbulence in shear layers, spray droplets, flash vaporization, primary and secondary atomization, mixing of chemical reactants, and liquid-gas interfaces. In addition, uncertainties in the characterization of the propellants at injection, including their mass flow rates, temperatures, and compositions, along with the uncertainties in thermomechanical laser parameters, play an important role in augmenting the unpredictability of the system. These effects lead to significant challenges for assessing the reliability of the ignition process.

The Center's simulation strategy is based on the construction of a large ensemble (millions) of simulations with different levels of physical fidelity that will be run on exascale class-machines. Task-based programming will be at the core of the computational developments using the language Regent in combination with a software compiler and runtime system called Legion, both of which were developed at Stanford University, to achieve more seamless performance from next-generation supercomputers. By taking advantage of task concurrency, hardware mapping, and statistical correlations, the technical breakthrough pursued here is to combine all the simulations to predict the reliability of laser-induced ignition in realistic operating conditions using a single ensemble run. The ensemble infrastructure also is used to enable distributed software verification, shared linear solver preconditioning, and general coupling techniques that steer and adapt the sampling of new ensemble members. The simulations will be validated by a tailored experimental campaign at the world-class rocket-testing facilities of Purdue University.

This project will expand the current state-of-the-art in the computational physics of fluid mechanics. For instance, fully resolved simulations of the combustor will push the boundary of available computing as a result of the wide range of temporal and spatial scales. Representation of the system dynamics at Kolmogorov scales will require up to 1 trillion grid points and millions of time steps. Furthermore, uncertainties in the system will require a large number of simulations to construct ignition probability maps. Critical elements that will be investigated to overcome these hurdles are (a) adaptivity in space and time and (b) multifidelity ensemble computations. Different strategies involving physical, numerical, and data-driven formulations will enable a companion effort at the University of Colorado at Boulder as part of this Predictive Science Academic Alliance Program III Center to introduce hundreds of low-cost, low-fidelity surrogate simulations (Figure 2). These will be executed in concert with high-fidelity simulations within the Legion Exascale runtime environment to enable the determination of the ignition success statistics.

Center for Predictive Engineering and Computational Science

University of Texas at Austin ✦ PIs: Dr. Robert Moser (rmoser@oden.utexas.edu) and Dr. George Biros (biros@oden.utexas.edu)

The Center for Predictive Engineering and Computational Science (PECOS) is a research center housed within the Oden Institute for Computational Engineering and Sciences at the University of Texas. The overarching goals of the Center's work through the Predictive Science Academic Alliance Program III are to (1) develop an advanced integrated predictive computational model for an inductively-coupled plasma (ICP) torch and use it to predict exit plasma properties and stable operating conditions, (2) develop advanced algorithms and performance portable programming tools to enable effective use of emerging exascale computing hardware and apply them to the simulation of the ICP torch, and (3) develop and apply advanced verification, validation, and uncertainty quantification tools for the ICP torch, including acquisition of required experimental data.

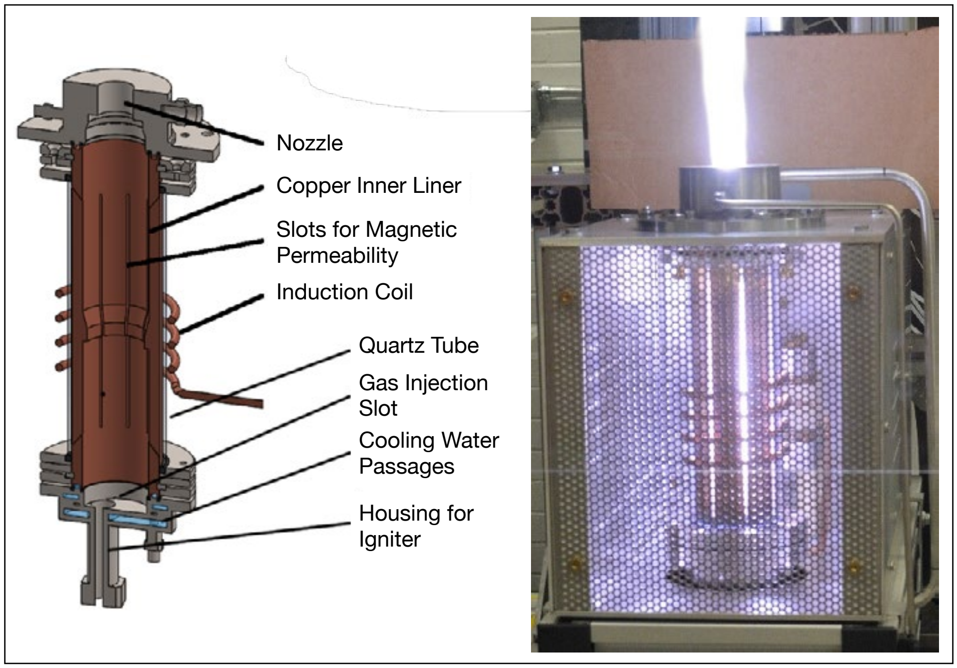


Figure 1. University of Texas plasma torch overview: cross-section of the plasma chamber (left) and torch in operation (right).

The torch of interest is a plasmatron system in which the plasma is produced in a cylindrical tube that is fed by a working gas at an inlet, in our case, either argon or air, and the hot effluents exhaust through an exit nozzle. The PECOS team has an experimental ICP torch facility locally that produces a relatively high-pressure plasma that has a wide variety of industrial and scientific applications including materials testing for thermal protection systems, gas pyrolysis, material synthesis, and coating deposition. The plasma it generates serves as a surrogate for plasmas in other applications in similar regimes.

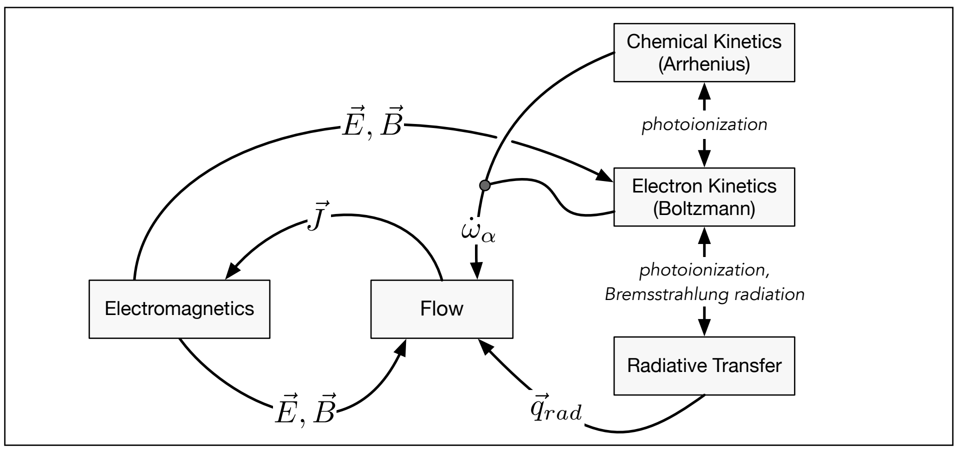


Figure 2. Overview of modeling schema mapping to underlying physics domains and primary coupling mechanisms.

The development of high-fidelity plasma torch simulations requires multi-physics coupling between a variety of phenomena and closure models including turbulent, compressible flow, thermal and chemical non-equilibrium gas dynamics, radio frequency electromagnetics, Boltzmann electron kinetics, and radiative transport. Generating reliable predictions of the ICP torch requires that all models and other assumptions be validated against relevant observations and that uncertainties be accounted for. To that end, the PECOS Center is engaged in a broad program to advance techniques for validation and uncertainty quantification (UQ). This program includes a focus on the development of algorithms for UQ analysis for problems described by expensive, high-fidelity models, the creation of lower fidelity surrogates and model decompositions for use in such algorithms, and development of techniques to design experiments that are maximally useful for validating predictive models.

Based on the physics involved, computational demands for full-scale plasma torch simulations are extremely demanding for even the largest supercomputers. To support efficient development and execution, the PECOS Center is engaged in advancing a variety of exascale-related technologies including the development of a performance portable runtime for heterogeneous computing. This runtime will provide rapid implementation, performance portability, and maintainability for the ICP torch simulator and other complex high performance computing applications. Another objective is to develop and evaluate computational algorithms and discretizations that perform well on emerging architectures for use in the ICP torch simulations and other applications.

Solution-verification, Grid-adaptation, and Uncertainty Quantification for Chaotic, Turbulent Flow Problems

University of Maryland ✦ PI: Dr. Johan Larsson (jola@umd.edu)

This Focused Investigatory Center is concentrating on the challenging problem of how to estimate errors and uncertainties in simulations of turbulent flows. These types of simulations are chaotic in nature and produce solutions with broadband spectra, two characteristics that make error estimation, error attribution, and uncertainty estimation particularly challenging. The Center is a collaboration between three principal investigators (along with Drs. Qiqi Wang at the Massachusetts Institute of Technology (MIT) and Ivan Bermejo-Moreno at the University of Southern California (USC)) and will provide primary support for five PhD students.

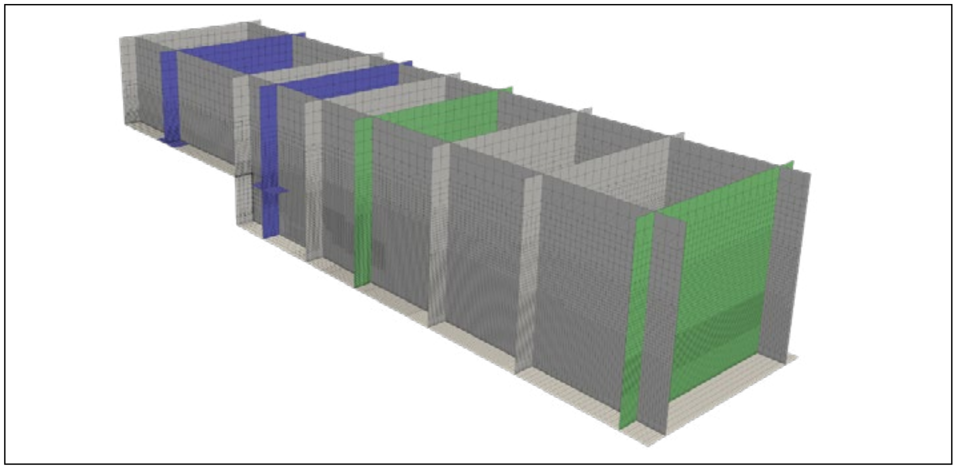


Figure 2. A computational grid for turbulence simulations produced by a grid-adaptation algorithm (i.e., without user input).

The high computational cost of turbulence simulations implies that sampling-based methods for uncertainty quantification often are not feasible. A useful alternative is the sensitivity of the problem, defined as the gradient of a Quantity-of-Interest (QoI) in the space of all uncertain or controllable parameters. The sensitivity can be computed efficiently (at a cost similar to a single turbulence simulation) using adjoint methods for non-chaotic problems. Chaotic problems, however, are, by definition, linearly unstable which implies that any infinitesimal perturbation will amplify exponentially. This frequently is termed the butterfly effect in popular culture, an example of which is seen in the top part of Figure 1 where the instantaneous solutions at different parameter values become uncorrelated to one another after some time. This linear instability makes the sensitivity computation mathematically ill-posed, since an infinitesimal parameter change will amplify without bound and produce an infinite gradient. This can be gleaned partly from the bottom of Figure 1, where the "noise" in the time-averaged QoI causes non-infinitesimal differences between parameter values that are infinitesimally close to one another.

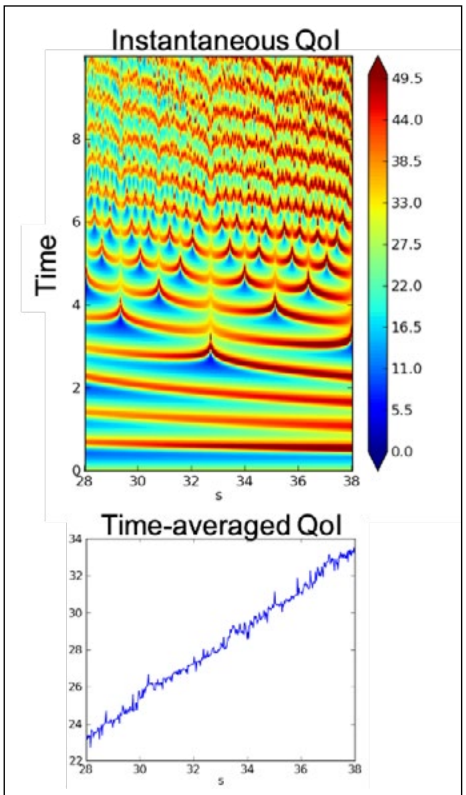


Figure 1. A sample Quantity-of-Interest (QoI) from the Lorenz system, illustrating the rapid de-correlation in time of nearby solutions (caused by differences in the parameters on the horizontal axis) which makes the problem of computing sensitivities of time-averaged QoIs an ill-posed problem (note the "noise" in the time-averaged QoI).

The main focus of the Center will be to develop methods for computing an approximate sensitivity gradient in a computationally-feasible manner. The Center will consider different approaches and then will assess and compare them on the main benchmark problem of turbulent flow over a flat plate with imposed pressure gradients. One approach will be to derive a mathematically-exact, regularized sensitivity and, then, to experiment with ways to reduce the required computational cost by introducing approximations. Another approach will be to use physics-inspired modeling to reduce (or even remove) the chaotic nature of the problem and, then, to use traditional adjoint methods to compute the sensitivity. In other words, the Center will consider both "sensitivity first, then modeling" and "modeling first, then sensitivity" approaches. The underlying assumption is that an exact computation of the regularized sensitivity will be too costly, even if theoretically possible.

The second focus of the Center will be on error estimation, specifically on estimating how the computational grid creates errors in the solution. The error estimates will be used both to estimate the error in the QoIs (when linked with the sensitivity gradient) and to drive grid-adaptation towards more optimal computational grids (an example is shown in Figure 2). The main problem in the context of turbulence simulations is the inherently broadband nature of the solution. Turbulence has a broad range of scales, and grid-refinement produces solutions with a broader range of scales. Mathematically, this means that a turbulence simulation is not in the asymptotic range of convergence which either invalidates, or at least makes questionable, standard error estimation techniques developed in the field of numerical analysis. The Center will attempt to overcome these problems by re-thinking the math and introducing some degree of physics-based thinking.

Center for Understandable Performant Exascale Communication Systems

University of New Mexico, Dr. Patrick G. Bridges (patrickb@unm.edu) ✦ University of Tennessee at Chattanooga, Dr. Anthony Skjellum ✦ University of Alabama at Birmingham, Dr. Purushotham Bangalore

Effective, next-generation scientific, engineering, and data-intensive applications demand communication systems that fully leverage available system resources for transformative scientific insight. Current high-performance computing (HPC) communication systems, however, are incremental outgrowths of systems from the era of single-threaded, reliable, general-purpose computing systems. Communication systems for emerging exascale applications must:

- ✦ Fully leverage available system resources such as heterogeneous processors, network offload, abundant parallelism, and complex memory systems;
- ✦ Handle the trade-offs between bandwidth, message rate, concurrency, and synchronization inherent in modern, highly-threaded architectures;
- ✦ Support continuous, reproducible evaluation and innovation in application, runtime system, and hardware design;
- ✦ Inform application scientists and system designers of communication system impact on performance.

Current HPC communication systems do not meet any of these requirements.

The overall mission of the Center for Understandable, Performant Exascale Communication Systems (CUP-ECS) is to meet the challenges of providing optimized, performance-transparent communication systems for emerging National Nuclear Security Administration (NNSA) exascale applications. The overall center goal is to provide new insights into both general-purpose and mission-specific NNSA applications, re-architect HPC application and system design, and yield transformative scientific insights across the breadth and depth of the NNSA mission. Our fine-grain approach, shown in Figure 1, spans three levels of innovation organized in a closed loop of iterative fundamental research, technical infrastructure innovation, and application/system assessment and evaluation.

Our research process is designed to address the overarching challenges facing modern communication systems through

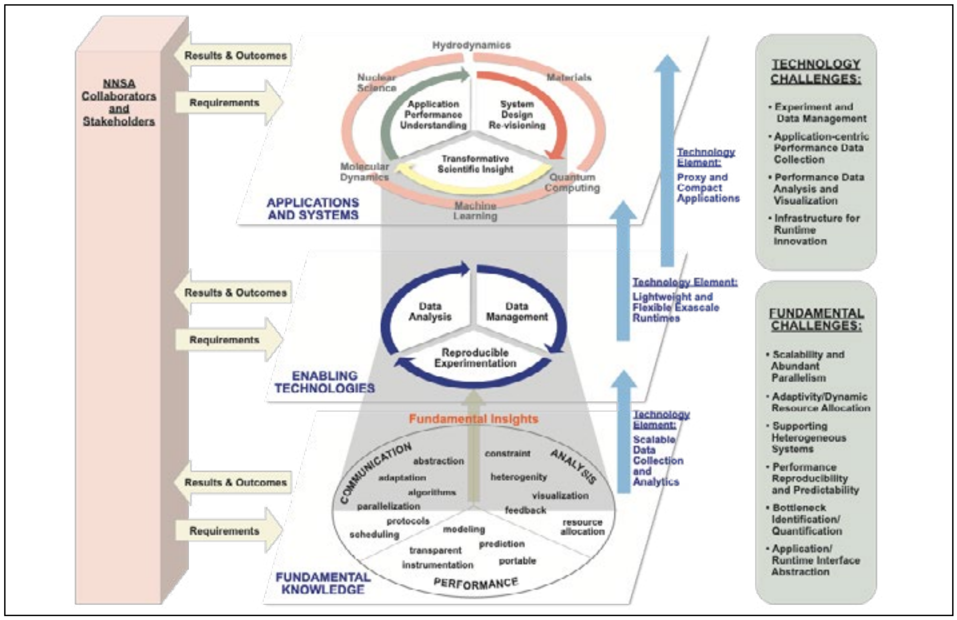


Figure 1. CUP-ECS's multi-level approach to fundamental communication system research, technical innovation and integration, and assessment in and on NNSA application and systems.

cycles of continuous research, integration, and assessment/evaluation in increasingly complex NNSA applications, as shown in Figure 2. Specifically, our research iteratively:

- ✦ Revisits and re-architects the relationship between exascale communication systems, applications, and hardware to support transformative scientific insights;
- ✦ Researches communication system innovations that accurately quantify, predict, abstract, and optimize exascale communication systems;
- ✦ Develops and integrates enabling technologies and leverage these fundamental research advances in support of NNSA applications and systems; and
- ✦ Continuously refines research, development, and system integration based on feedback.

Relevance, value, and impact to NNSA for exascale applications and systems will be demonstrated via NNSA proxy applications as well as production applications. Primary research will prototype communication innovations in existing and, if necessary, newly-developed proxy applications and will work with NNSA personnel to integrate and evaluate research results production applications. Center personnel will

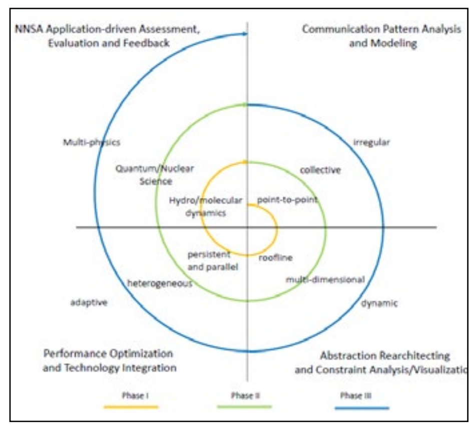


Figure 2. CUP-ECS research process.

design, develop, and optimize new communication abstractions, models of their performance, and perform roofline-style constraint analyses of their impact to NNSA application performance. These innovations and insights then will be employed to provide actionable insights to NNSA application and runtime designers. Our results will help designers understand, predict, and optimize key trade-offs between application communication strategies and application performance. Systematically assessing the impact of these insights to NNSA applications then will lead, in turn, to yet newer runtime abstractions and optimizations that further improve application performance, resulting in the next iteration of models, assessment, and innovation.

Minority Serving Institutions Partnership Program

Overview

David Canty, Federal Program Manager, National Nuclear Security Administration (david.canty@nnsa.doe.gov)

The Minority Serving Institutions Partnership Program (MSIPP) is designed to build a sustainable pipeline between minority serving institutions (MSIs) and the nuclear security enterprise in disciplines of science, technology, engineering, and mathematics (STEM).

MSIPP continues to drive towards the National Nuclear Security Administration's Strategic Vision Mission Priority #4 to strengthen key science, technology, and engineering capabilities through its enduring STEM pipeline with MSIs, supporting students ranging from K-12 to the postdoctoral level.

MSIPP supports MSIs through competitive, consortia-based grant awards with a 3-5 year period of performance. Through the consortia, MSIPP invests in a diverse portfolio including various student enrichment programs (career days, externships, internships, industry days, short courses), curriculum development, laboratory development, joint research efforts, and STEM outreach programs. Students are provided with internship opportunities across the enterprise that are in direct alignment with their academic disciplines. These internships prepare students to make significant and immediate contributions to the nuclear security enterprise upon graduation.

Consortia in the Minority Serving Institutions Partnership Program

- Advanced Manufacturing Network (AMFN), American Higher Education Consortium, Lead
- Additive Manufacturing Post Processing Partnership (AMP3), University of the District of Columbia, Lead
- Advanced Sensors Technologies for Applications in Electrical Engineering - Research and Innovation eXcellence Consortium (ASTERIX), Florida International University, Lead
- Consortium for High Energy Density Science (CfHEDS), Florida A&M University, Lead
- Consortium Hybrid Resilient Energy Systems (CHRES), SUAGM, Inc. dba Universidad Ana G. Méndez-Gurabo, Lead

- Consortium on Nuclear Security Technologies (CONNECT), University of Texas, San Antonio, Lead
- Energy Sciences: Experimental and Modeling (ESEM), Prairie View A&M University, Lead
- Consortium for Nuclear Security Advanced Manufacturing Enhanced by Machine Learning (NSAM-ML), North Carolina Central University, Lead
- Partnership for Proactive Cybersecurity Training (PACT), University of Arizona, Lead
- Partnership for Research and Education Consortium in Ceramics and Polymers (PRE-CCAP), University of Arizona, Lead
- Pipeline Development of Skilled Workforce in STEM through Advanced Manufacturing (STEAM), North Carolina A&T University, Lead
- Successful Training and Effective Pipelines to National Laboratories with STEM Core (STEP2NLs), North Carolina A&T University, Lead
- Scholarly Partnership in Nuclear Security (SPINS), Alabama A&M University, Lead

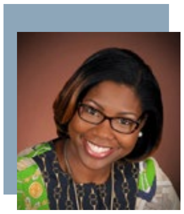
Minority Serving Institutions

Alabama A&M University
Bay Mills Community College
Board of Regents Nevada System of Higher Education
Cankdeska Cikana Community College
Elizabeth City State University
Florida A&M University
Florida International University
Howard University
Inter-American University of Puerto Rico - San German
Miami Dade College
Morehouse College
Morgan State University
Navajo Technical University
New Mexico State University
North Carolina A&T State University
North Carolina Central University
Prairie View A&M University
Salish Kootenai College
Southern University of Baton Rouge
Southern University of New Orleans
St. Mary's University
SUAGM, Inc. dba Universidad Ana G. Méndez-Gurabo
Tennessee State University
Turtle Mountain Community College
University of Arizona
University of California Merced
University of New Mexico
University of Puerto Rico, Mayaguez
University of Puerto Rico, Rio Piedras
University of Texas at El Paso
University of Texas at San Antonio
University of the District of Columbia
Virginia State University

Lab/Plant Partners

Argonne National Laboratory
Brookhaven National Laboratory
Kansas City Plant
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
National Energy Technology Laboratory
Oak Ridge National Laboratory
Pacific Northwest National Laboratory
Sandia National Laboratories
Savannah River National Laboratory
Y-12 Plant

Alta C. Bailey, Kansas City National Security Campus and Oak Ridge National Laboratory (abailey@kcns.doe.gov)
Years at KCNSC: September 2018-Present ✦ **Years at ORNL:** February 2017-June 2017, May 2016-August 2016
Degree: MA, BS, Chemical Engineering (2018, 2013) ✦ **Years in MSIPP**: 2016-2018, North Carolina A&T State University



Early in my career as a process engineer for a large, consumer products company, I came to the realization that if I could be a part of the upstream technology conceptualization and development process for manufacturing, I could implement the changes and improvements needed to best support the hardworking technicians. This realization motivated me to return to graduate school to narrow my focus and gain more research experience. In the fall of 2015, I entered the graduate Chemical Engineering (ChemE) program at North Carolina A&T State University to earn an MS (Figure 1). At that juncture, I had no idea that this path would lead me to the Kansas City National Security Campus (KCNSC), supporting our Nation's security.

In my spring semester after searching for a thesis research topic and recognizing there weren't many opportunities available in my department, I contemplated switching to a coursework-only degree. Unbeknownst to me, the MSIPP's Consortium of Additive Manufacturing (CAM) was seeking a ChemE graduate student to collaborate on a project with Oak Ridge National Laboratory (ORNL). Dr. Shamsuddin Ilias, my separations and transport phenomena professor, presented me with the opportunity, and, about a week later, I attended an MSIPP university-led workshop. There I met Dr. Amelia Elliott from ORNL's Manufacturing Demonstration Facility (MDF). The MDF serves as a hub between equipment manufacturers, end users, and researchers to advance state-of-the-art technologies and to revolutionize the way products are designed and built using a wide array of additive manufacturing (AM) technologies.

I've always known about Sandia National Laboratories, as they've recruited at my university for years. However, I never knew that other Department of Energy laboratories existed. During my two internships at ORNL's MDF, I was mentored by a corporate fellow, worked alongside some of the most talented experts in electron microscopy and AM, completed research towards my master's thesis, submitted a conference paper, and presented at the 27th Annual International Solid Freeform Fabrication Symposium in Austin, Texas. All of this was possible through MSIPP, and it was at a university-led workshop where MSIPP Program Manager, Amy Moser, recognized in me the talent and skill set KCNSC was looking for and urged me to apply. After applying, accepting the offer, and defending my thesis, I moved almost 1,000 miles across the country to Kansas City, Missouri.

"In my two short years at KCNSC, I can say that I've not only been stretched beyond my degree's traditional boundaries, but also I've been challenged to build my skill set in multiple areas where I had no prior experience. Coming in I knew, through candid conversations had with KCNSC employees supporting MSIPP, that this was a place where I was going to be technically challenged, professionally developed, and supported to become my best self."

KCNSC welcomed me in September 2018, and I have worked in both the metal AM and advanced technology development departments. I have supported standardization, qualification, and baseline development activities for metal AM design and use. Partnering with internal departments and outside vendors, I established a framework for the use and build of mechanical test specimens across two departments and led laboratory analysis efforts used to validate predictive melt pool models for selective laser melting parameter tuning. My work involved cross-functional engagement with modeling and simulation and our engineering laboratories. In my current role, I support the onboarding of new electronics technologies, methods, and approaches to traditional manufacturing methods and early-stage development for printed electronics, serving as the point of contact for Drop-On-Demand ink jet technology.

Figure 1. Alta Bailey, a former MSIPP graduate researcher, transporting a glass graduated cylinder across an NC A&T university mechanical engineering lab for later use. Alta received two lab appointments through the Higher Education Research Experiences (HERE) program with MSIPP partner, ORNL. While there, she developed a bench scale method for incorporation and testing of the in-site use of nanoparticles within the AM technology, binder jetting. She joined the Kansas City National Security Campus in late 2018 after graduating from NC A&T with her MS in Chemical Engineering."

In my two short years at KCNSC, I can say that I've not only been stretched beyond my degree's traditional boundaries, but also I've been challenged to build my skill set in multiple areas where I had no prior experience. Coming in I knew, through candid conversations had with KCNSC employees supporting MSIPP, that this was a place where I was going to be technically challenged, professionally developed, and supported to become my best self. Through MSIPP I've been fortunate to work at the KCNSC.

Imani S. Ballard, Kansas City National Security Campus (iballard@kcnsc.doe.gov)
Years at KCNSC: Staff: July 2020-Present, **Intern:** May-August 2015 ✦ **Degree:** BS, Mechanical Engineering (2017) ✦ Years in MSIPP: 2014-2017, Howard University

I have always known about my affinity towards science, technology, engineering, and mathematics (STEM). I spent my four years of high school in the engineering magnet program learning how to manipulate three-dimensional (3D) models, understand structures, and even performed a senior design project. During my senior year in high school, I decided that I would attend Howard University in Washington, DC, one of the most prestigious Historically Black Colleges and Universities (HBCU) in the country. With this decision came Howard's private institution tuition. Although they offered me a partial academic scholarship, I really didn't want any student loans. I ended up reaching out to the university's softball coach to see if there was an opportunity for a partial athletic scholarship. The next thing I knew, I was pursuing a Mechanical Engineering Degree as a National Collegiate Athletic Association (NCAA) Division I student athlete.

During my first semester, my computer-aided design (CAD) professor and both of the teaching assistants noticed my affinity for 3D modeling. They offered me a position as a paid summer camp counselor for their CAD camp for the middle school on campus. I took the position and was required to teach seventh and eighth grade students CAD processes and have them develop a camp design project. I then attended the 2014 Model-Based Enterprise Workshop at the Kansas City National Security Campus (KCNSC). It was there where I really found out about the mission of the Minority Serving Institution Partnership Program (MSIPP) and the Nuclear Weapons Enterprise (NWE).

I fell in love at first sight with the KCNSC mission, their dedication to reducing their carbon footprint, and their culture. I spoke with all of the subject matter experts and managers present at the workshop trying to figure out how to apply for an internship. I never will forget the call I received to schedule my phone interview. That phone call was only topped by the call I received after the onsite interview offering me an internship with Honeywell at the KCNSC.

"Without MSIPP, I never would have had the opportunity to showcase my talent within the NWE, and for that I will be forever grateful. Fortunately, my work with MSIPP is not over.

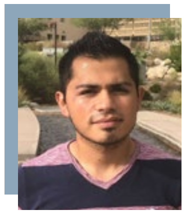
As a full time employee, I am fortunate enough still to be a part of this revolutionary program. I now lead the MSIPP Alumni Program at the KCNSC whose goal is to aid in the transition to Kansas City and the KCNSC by providing a myriad of resources that develop personal and professional skills."

I ended up having two internships at the KCNSC. My first internship was with the Advanced Engineering, Simulation, and Analysis department. I was fortunate enough to participate in the development of a database that is being used currently across our Model-Based Enterprise (Figure 1). This internship was directly funded through MSIPP. My second internship was funded by Honeywell in their materials organization. After my second internship, I was offered a full time position in the materials organization working on Chemically Vapor Deposited Thin Films and researching new protective coatings. As a full time employee, I have had a hand in replacing carcinogenic materials, introducing new coatings into production, and developing a completely new material that is easier for our facility to manipulate and use. Without MSIPP, I never would have had the opportunity to showcase my talent within the NWE, and for that I will be forever grateful. Fortunately, my work with MSIPP is not over.

Figure 1. Imani Ballard preparing a Design of Experiments tribological test for a Plasma Enhanced Chemical Vapor Deposited Diamond Like Carbon Coating (PECVD DLC) technology insertion study. She joined the Kansas City National Security Campus (KCNSC) mid-2017 after two internships at said facility and graduating from Howard University with her BS in Mechanical Engineering.

As a full time employee, I am fortunate enough still to be a part of this revolutionary program. I now lead the MSIPP Alumni Program at the KCNSC whose goal is to aid in the transition to Kansas City and the KCNSC by providing a myriad of resources that develop personal and professional skills. MSIPP has allowed me to become a Soft Skills for STEM Young Professional where I have had the privilege of speaking at multiple professional development workshops. I have traveled across the country to tell my story to other students attending my alma mater and other HBCUs. Students who have talked to me see how the National Nuclear Security Administration realized that there was a racial disproportionality in their enterprise and appreciated how they used MSIPP as one way of addressing it. Sharing my story has shifted the minds of current Minority Serving Institutions students, allowing them to reconsider where and how they want to use their talents. Being able to assist and mentor other students in the MSIPP consortiums has been the highlight of my MSIPP journey.

Luis Angel Chavez Atayde, Los Alamos National Laboratory (luis_chavez@lanl.gov)
Years at LANL: June 2019-Present ✦ **Degree:** PhD, Mechanical Engineering, University of Texas at El Paso ✦ **Years in MSIPP**: 2019-2020



I am currently working in several multidisciplinary projects Los Alamos National Laboratory as a postdoctoral research associate in the Materials Synthesis and Integrated Devices group. The focus of these projects is to explore and devise ways to increase the efficiency of clean energy conversion systems to make them viable for multiple applications, as well as detect any failures within said systems to reduce loss in performance and downtime.

My first interaction with the laboratory was thanks to a collaboration between my university and the laboratory through a Minority Serving Institution Partnership Program (MSIPP). One of the projects that I am currently working on was partially made possible thanks to the opportunity that I had by being part of the Partnership for Research and Education Consortium in Ceramics and Polymers (PRE-CCAP) and a summer internship at LANL. During that internship, I was able to help come up with new ideas and methods to potentially improve the efficiency of fuel cell systems. The results from the research performed during that summer internship led to securing funding from the laboratory to convert these ideas into a laboratory-funded project. The projects that I have had the opportunity to contribute in have the potential to greatly advance the energy and energy security sectors, which will benefit both society and my future career. In addition to the research experience that I got from this opportunity, I was also able to access a strong network of world-renowned researchers and scientists, as well as secure an opportunity to keep learning from these people and continue my training as a researcher.

"During that internship, I was able to help come up with new ideas and methods to potentially improve the efficiency of fuel cell systems. The results from the research performed during that summer internship led to securing funding from the laboratory to convert these ideas into a laboratory-funded project. The projects that I have had the opportunity to contribute in have the potential to greatly advance the energy and energy security sectors, which will benefit both society and my future career."

I decided to join LANL as a postdoctoral research associate because of the extremely beneficial learning experience, the intellectual challenge that represents working and interacting with the top scientist in this field, as well as this valuable opportunity to help evolve the field of sustainable energy and energy security and create a positive impact in this country and the world.

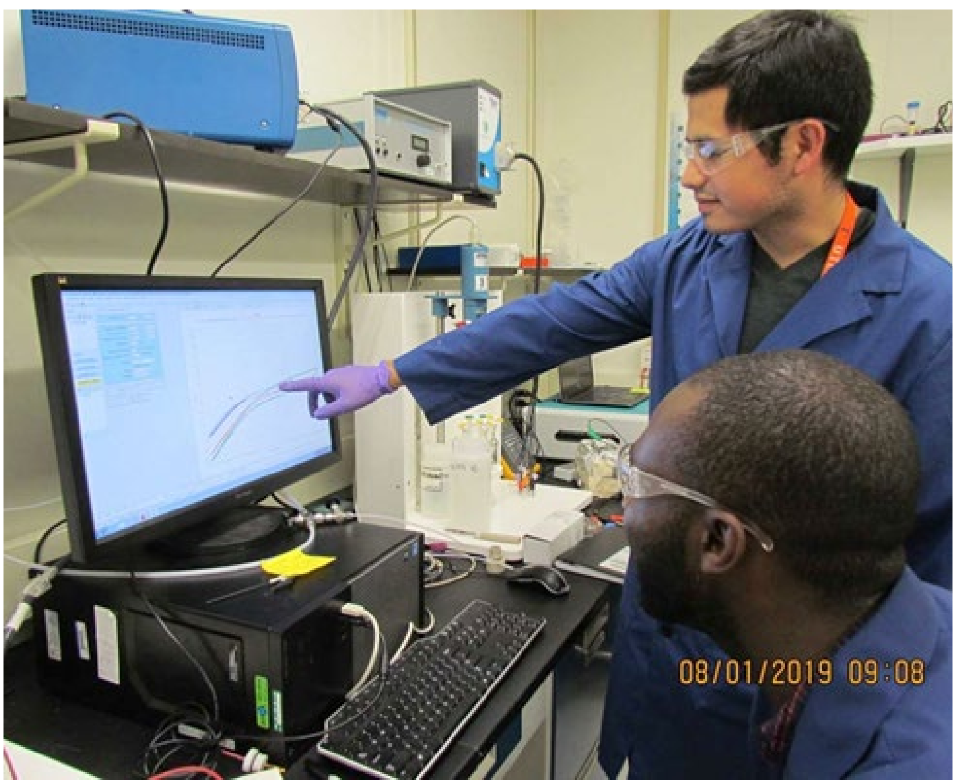
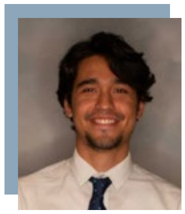


Figure 1. Luis working with fellow MSIPP student on data analysis of a novel energy conversion methods.

Luis Delfin (delfin@lanl.gov)
Degree in Progress: BS, Mechanical Engineering, University of Texas at El Paso ✦ **Advisor:** Dr. Yirong Lin ✦ **MSIPP:** 2019-Present

Research Topic
Additive Manufacturing of Functional Ceramics (UTEP), Polymer and Energy-related Research (LANL)



Research Responsibilities
As a post-baccalaureate student with the Smart Materials Processing Lab Group at Los Alamos National Laboratory (LANL), I am contributing to the work on the synthesis and characterization of novel polymers materials and to the design and development of new hardware for sensing devices. I will be starting my PhD at Stanford University after completing my post-baccalaureate at LANL.

Benefits of MSIPP
MSIPP has given me the opportunity to experience working at a national laboratory. While at LANL, I have had the opportunity to work with state-of-the-art equipment and to learn from scientists who are world leaders in their field. This type of exposure has continued to inspire my desire to achieve a graduate degree and career in a science, technology, engineering, and mathematics fields.

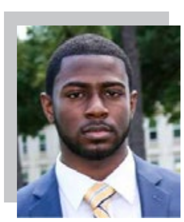
National Laboratory Experience
MSIPP gave me an opportunity that I might not have encountered otherwise. I had the opportunity to start my career in research early during my undergraduate studies. I worked in the Smart Materials Processing Lab Group, making me a better mechanical engineering student. I am certain that MSIPP's opportunity to start my research career contributed immensely to my getting accepted into Stanford's Material Science and Engineering program. Now, MSIPP has provided the opportunity to continue my research career as a post-baccalaureate student at LANL, and this has made graduate school less intimidating. I have had the opportunity to interact with scientists from different backgrounds, allowing me to become a well-rounded researcher. At LANL, I have started working with fuel cells, where I have synthesized novel polymers and sensors. I have learned about various characterization techniques to better understand the materials that I synthesized in the lab. More importantly, I have gained the communication skills to properly present scientific findings in a professional setting. I am grateful that my mentors encourage me to develop new ideas every time we discuss our research progress. LANL has given me the tools necessary to expand my knowledge and thrive in the field of materials science.

I have been learning about complex research topics from the best of the best. Also, I have had the opportunity to attend interesting webinars hosted by the laboratory presented by faculty from around the world.

During the summer, I was tasked with mentoring and teaching 15 students about three-dimensional (3D) modeling and different additive manufacturing techniques. I developed a curriculum for 10 weeks and presented the fundamentals of 3D printing and computer-aided design. I also assigned projects and homework that aided students to fully grasp the concepts. This was a great opportunity for me to develop skills that I will need as a professor. This post-baccalaureate experience will have a great impact on my future career, as it opens the opportunity to return to the laboratory as a postdoctoral researcher to further my professional development.

André Spears (ajspears@lanl.gov)
Degree: PhD, Nanoscience and Microsystems Engineering, University of New Mexico ✦ **Advisor:** Dr. Fernando Garzon ✦ **MSIPP:** 2012-Present

Research Topic
Probing the Impacts of Ultra-Low Platinum Loadings on Membrane Degradation Mechanisms



Research Responsibilities
I conduct research in an unexplored area of science and contribute to a knowledge-base in order to improve the fundamental understand of energy-related research. I prepare samples for testing and analysis and characterize samples before and after testing.

Benefits of MSIPP
Through MSIPP I have been introduced to research and have been able to network with scientists in various fields. I also received financial support throughout my education.

National Laboratory Experience
I attended Southern University and A&M College and was introduced to Los Alamos National Laboratory (LANL) through a relationship established by MSIPP. The MSIPP provided me the opportunity to conduct research at LANL. I enjoyed my first summer experience at LANL and was very enthusiastic about working with their staff. The following summer I returned and became more immersed in exciting research. As a result, I considered pursuing a graduate degree. Through relationships developed by my mentors, I eventually met my future graduate school advisor, a former LANL staff scientist turned professor. This connection may not have been possible without the support of MSIPP. My career trajectory changed after the experience of working at LANL.

In 2016, I was accepted into graduate school at the University of New Mexico and began research. I maintained my relationship with LANL and was accepted into the African American Partnership Program. After completing my course requirements, I was allowed to conduct my thesis research at LANL as a graduate research assistant. While at LANL, I worked on projects that allowed me to expand my understanding of research science.

In the past six years, MSIPP has positively impacted my life. It has helped to guide my career path. I defended and passed my doctoral defense on December 9, 2020. This is something that I never imagined but that was made possible by the National Nuclear Security Administration. More recently, I was offered a postdoctoral position at LANL. If it had not been for MSIPP, I would not have these career path opportunities.

Juanita P. Stephen (jstephen@kcnsc.doe.gov)
Degree in Progress: MS, Mechanical Engineering, Virginia Polytechnic Institute and State University ✦ **Advisor:** Dr. Reza Mirzaeifar ✦ **MSIPP**: 2015-Present

Research Topic

Experimental and Numerical Analysis of Process Parameter Effect on Mechanical Properties and Microstructure of Additively Manufactured 316L Stainless Steel

Research Responsibilities

My research responsibilities include the use of a combined computational and experimental framework to investigate the interaction between process parameters, microstructure, and mechanical properties of three-dimentionally printed 316L stainless steel alloys.

Benefits of MSIPP

The Minority Serving Institution Partnership Program (MSIPP) gave me the opportunity to be where I am today. I was able to participate in summer research experiences at various universities, and I was the first Lincoln University (LU) student who was recruited by Kansas City National Security Campus (KCNSC) to be an intern as well as receive the first place KCNSC MSIPP Scholarship.

After completing my first internship and beginning my graduate program at Virginia Tech, I was the first MSIPP student for whom the KCNSC coordinated a student project. MSIPP provided the path to allow me to accept a full-time offer at KCNSC.

Networking Opportunities

Being introduced to new people and opportunities for the first time can be exciting; and college was full of firsts. I was the first in my immediate family to leave California, and attend college at LU in Missouri, majoring in mathematics. Towards the end of my freshman year, Ms. Stallings, a math professor and principal investigator for MSIPP, approached me about a MSIPP sponsored summer exchange at Howard University focused on additive manufacturing (AM). Through this experience I decided to pursue a career in mechanical engineering (ME), there was just one problem; I wanted to complete my mathematics degree at LU and they didn't have an ABET accredited ME program.

While continuing my courses, I led a program called LU-IN-STEP geared towards preparing students for careers in science, technology, and engineering. On one occasion, we visited KCNSC, where I was intrigued by the culture, and was determined to intern there. Through MSIPP, I was provided an avenue to explore my interest in ME while being introduced to numerous career opportunities and people that I would not have been exposed to otherwise. As a conference attendee, I presented on topics related to AM Glass to Metal Seals and Nondestructive Testing.

During my senior year, I became the first LU student accepted for a summer internship at KCNSC due to the pipeline MSIPP developed. During my three internships, I met other interns and professionals, built my technical knowledge, and returned to LU to teach an AM camp. Subsequently, I was awarded the first place KCNSC MSIPP scholarship, and met the MSIPP federal program manager and leadership team.

Upon completion of my bachelor's degree, I enrolled at Virginia Tech to obtain a master's degree in ME where I will graduate December, 2020, and then begin a full time position at KCNSC. All of which, would not be possible without the continued support from MSIPP.

Stefan Williams (stefanw@lanl.gov)
Degree in Progress: PhD, Chemical Engineering, The University of Tennessee ✦ **Advisor:** Dr. Thomas A. Zawodzinski Jr. ✦ **MSIPP**: 2015-Present

Research Topic

The Controlled Synthesis of Hydrogen Electrocatalysts for Alkaline Exchange Membrane Fuel Cell and Electrolysis Applications via Chemical Vapor Deposition

Benefits of MSIPP

MSIPP has provided me financial support and a unique opportunity to accelerate and enhance my research by having access to state-of-the-art facilities and various characterization techniques found at the national laboratories.

National Laboratory Experience

My journey with the MSIPP began months before I graduated from Morehouse College in the Spring of 2015. I was approached by the chair of the Physics Department who asked what my post graduate plans were. He offered me a summer internship opportunity at Los Alamos National Laboratory (LANL). Without hesitation, I accepted, not knowing the impact that that decision would have on my future. As a 2015 summer intern, I worked in the Consortium for Materials and Energy Security which is sponsored by MSIPP. My research focused on general electrochemistry with applications for hydrogen fuel cells. During the three months of my internship, my outlook on the efficacy of my degree changed. I continued at LANL as a post-baccalaureate student in the Winter of 2016.

During this time, I collaborated with several principal investigators in the Materials Physics and Application group on research topics ranging from fuel cell hardware and membrane durability to hydrogen fuel quality standards and sensors development. Being surrounded and trusted by successful scientists gave me the confidence to pursue higher education. I became a second-generation mentee at The University of Tennessee, Knoxville in the Chemical and Biomolecular Engineering Department in the Fall of 2017. I earned my MS degree with a concentration in Chemical Engineering in the Spring of 2019 and expect to graduate with my PhD in 2021.

While at The University of Tennessee, I was accepted into LANL's African American Partnership Program. Through opportunities afforded by MSIPP and LANL, I have gained confidence not only in my research but also in me. Because of the impact of MSIPP on my life, I plan to pursue a career in academia. In this way, I plan to inspire other students, like me, who are uncertain about their abilities. I plan to promote them to gain confidence and pride in who they are and what they can accomplish. MSIPP helped facilitate my interest in science, technology, engineering, and mathematics (STEM) and in the opportunities that STEM can provide.

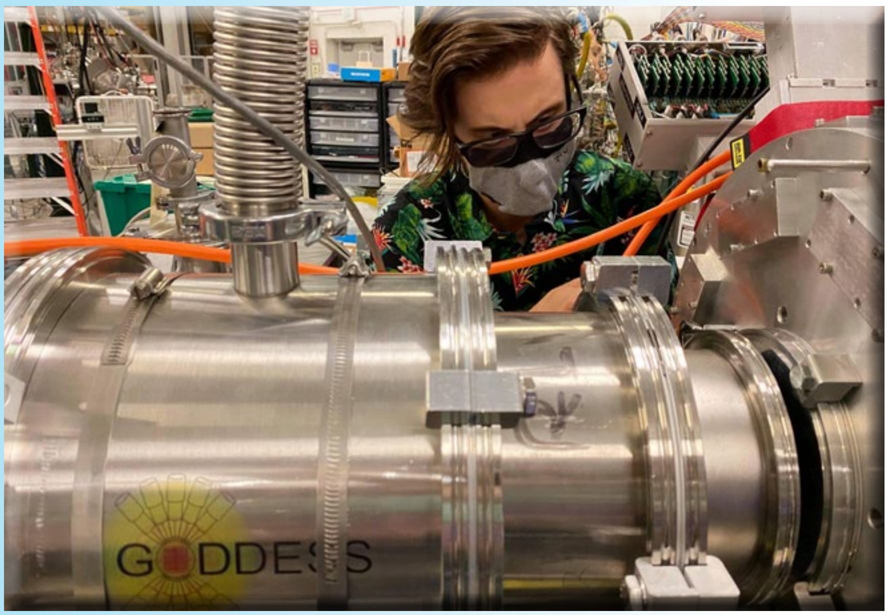
"On one occasion, we visited KCNSC, where I was intrigued by the culture and was determined to intern there. Through a pipeline developed by MSIPP, I was provided an avenue to explore my interest in [mechanical engineering] while being introduced to numerous career opportunities and people that I would not have been exposed to otherwise."

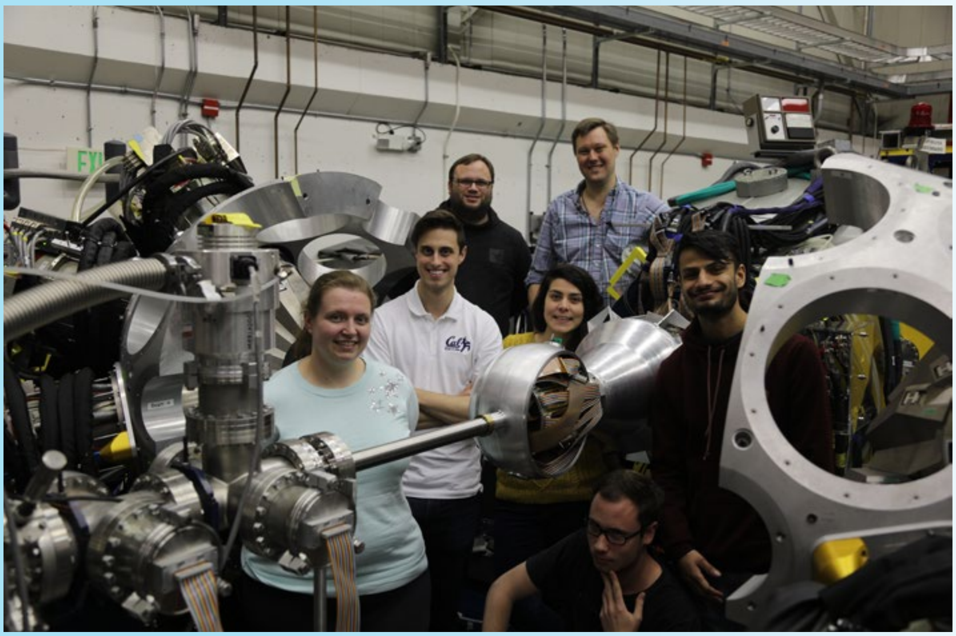
— Stefan Williams
Los Alamos National Laboratory

"MSIPP helped facilitate my interest in science, technology, engineering, and mathematics (STEM) and in the opportunities that STEM can provide."

— Juanita P. Stephen
Kansas City National Security Campus

Fellowship Programs





Experimenters (front: Harry Sims of Rutgers University; middle row, from left: Heather Garland, Chad Ummel and Gwen Seymour, all of Rutgers University, and Rajesh Ghimire of the University of Tennessee–Knoxville and Oak Ridge National Laboratory; and back row, from left: Josh Hooker of UTK and Steven Pain of ORNL) pose with the ORRUBA and GRETINA detector arrays, coupled together to form GODDESS. Photo cedit: Andrew Ratkiewicz/Oak Ridge National Laboratory, U.S. Dept. of Energy

Sylvia Hanna searches for single crystals of actinide metal-organic frameworks under a microscope.

Teresa Bailey, Lawrence Livermore National Laboratory (bailey42@llnl.gov)
Years at LLNL: February 2008-Present ✦ **Degree:** PhD, Nuclear Engineering ✦ **CSGF:** 2002-2006, Texas A&M University

The Department of Energy/National Nuclear Security Administration (DOE/NNSA) Computational Science Graduate Fellowship (CSGF) is a unique program that prepared me well for my career at Lawrence Livermore National Laboratory (LLNL). During the fellowship, I had practica at LLNL, Oak Ridge National Laboratory, and Los Alamos National Laboratory (LANL), giving me a good overview of national laboratory missions and team culture. During my career, I've used the relationships I developed to support efforts that are important to the nation, and the expertise and network that I established have helped all three laboratories.

I have had four main jobs as an LLNL employee. From 2008 to 2015, I was a staff member working on deterministic transport algorithm development with a focus on massively parallel algorithms. I used my numerical method expertise to understand code behavior and to make recommendations to improve methods within the code. In these efforts, collaboration was crucial, and I had a chance to work closely with other staff at LLNL, LANL, and Sandia National Laboratories staff and with university partners. Together we built a strong understanding of the theory and development necessary to make key algorithms scalable. It was a great introduction to the power of teamwork for me, a lesson I take to heart to this day. Many NNSA laboratory projects learned from this collective effort, producing significant benefits for production codes.

At LLNL, we used this project to successfully port our production code to Sequoia, realizing excellent scaling on more than a million message-passing interface tasks—a feat considered a grand challenge problem at the time. The project established a new production code that has become a lab standard.

My DOE CSGF-based education prepared me well for these multidisciplinary projects. It helped me develop an excellent background in numerical methods and provided entry-level knowledge of parallel algorithms, both of which were vital. The practicum experience helped me foster collaborations I relied on for the job.

Figure 1. The Sierra supercomputer provides a big challenge for my teams and me. We enjoyed tackling this grand challenge together."

From 2015 to 2020, I became deterministic transport project lead, guiding other LLNL transport experts to build a new project at LLNL from the ground up. This was my first foray into leadership at the laboratory, one that reinforced the importance of team. I realized quickly that we could only succeed together, and I was blessed to work with some truly amazing colleagues. Together, we achieved significant growth and collaborated to tackle major technical challenges.

This project had two major goals: (1) establish a research path for high-order finite element discretization applied to the deterministic transport thermal radiative transfer application space, and (2) achieve significant computational performance gains on Sierra, a heterogenous architecture that is fundamentally different from Sequoia. As a team, we met both goals. LLNL's deterministic transport team has successfully ported two production transport codes to Sierra and achieved significant, game-changing performance gains.

In this part of my career, I used numerical methods expertise gained from DOE CSGF-approved courses. I led the construction of a multi-disciplinary team of mathematicians, computer scientists, and nuclear engineers to solve these problems—mirroring elements of the DOE CSGF program of study. LLNL deterministic transport has been successful, because we built a high-functioning, multi-disciplinary team.

In 2016, I took on additional responsibility as a project leader in the area of Nuclear Science, helping to steer nuclear physics at LLNL in the areas of experiment, theory, evaluation, and processing making all the pieces connect into a comprehensive capability. The job expanded my view of predictive science, because I learned how material models are developed from start to finish. It offered a new opportunity to build collaborations within LLNL, with other DOE laboratories, and with universities.

In 2020, I took on an entirely new job as the National Stockpile Program Group Leader. My role is to oversee physics activities associated with LLNL's Annual Assessment Review and the Independent Nuclear Weapons Assessment Program. This role has changed my perspective, as I have become a consumer of computational tools instead of a developer of one.

DOE/NNSA laboratories are on the cutting edge of applying high performance computing (HPC) to problems of national and international significance. Not only does NNSA procure state-of-the art HPC platforms, it also develops production software that runs well on these platforms. We use this capability every day to solve our programmatic problems.

As part of a DOE/NNSA laboratory, I have had the opportunity to work with computer vendors, universities, other national laboratories spanning NNSA and the DOE Office of Science, and my own world-class LLNL collaborators. At LLNL, we feel tremendous pride and responsibility in our national security work, and teaming across disciplinary lines is how we solve extremely complex problems. CSGF was excellent for me because it got me to start thinking about the multidisciplinary nature of computational science, which is exactly what we do at LLNL to achieve solutions to our grand challenge problems.

Miriam Kreher (mkreher13@gmail.com)
Degree in Progress: PhD, Nuclear Engineering, Massachusetts Institute of Technology ✦ **Advisor**: Dr. Benoit Forget ✦ **CSGF**: 2017-Present

As a nuclear engineer, I could not have asked for a more practical experience than working at a national laboratory. The Department of Energy runs an amazing suite of nuclear research, from hands-on experiments to top-of-the-line simulations. Even though I am a computational scientist, my time at Los Alamos National Laboratory (LANL) has allowed me to witness firsthand nuclear criticality experiments at the Nevada Test Site and to talk to the people building the next space reactor. All of this puts my work into perspective. There is something thrilling about seeing a product emerge from my everyday modeling work. In my practicum at LANL, I developed a tool that allows reactor designers to model, optimize, and quantify the error on their reactor designs, specifically in time-dependent simulations. As soon as I had a viable code, I had a user. Not only did I get beta-testing feedback immediately, but I was excited to do work that someone needed as soon as possible.

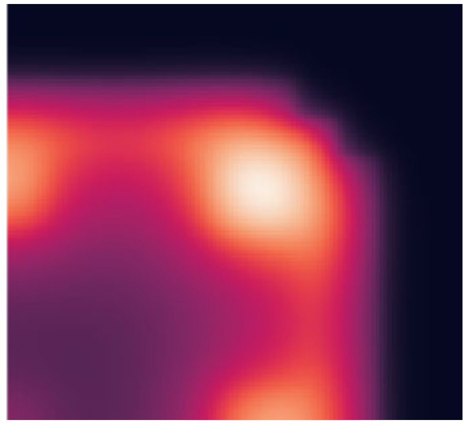


Figure 1. shows the power distribution in a quarter-core of a test reactor. I built this simulation from a time-dependent neutronics benchmark, and I use it to test and compare various numerical methods that can be useful in the transient simulation of reactors.

The practicum and the complete flexibility over my thesis topic were the two most important reasons why I accepted the CSGF over other prestigious fellowships that I was offered. Thanks to the fellowship, I had complete flexibility in choosing my PhD topic, so I picked what sounded like the most interesting and challenging problem I could think of. While it hasn't been easy, I have been continually motivated by the impact I am having in the nuclear field.

I have focused my research on the transient simulation of nuclear systems using Monte Carlo codes. Monte Carlo, cleverly named after the famous casino, is the state-of-the-art simulation tool for neutron transport. In Monte Carlo, neutrons are modeled individually, and every single interaction is based on a probability distribution - like a game of chance! Although it is the most accurate tool available, it is very computationally expensive, even more so when it is coupled to other codes such as thermal hydraulic solvers. Nonetheless, since most existing nuclear reactors are large neutron systems surrounded by hot water, it is imperative to model coupled neutronics and thermal hydraulics. My work is focused on the development of numerical methods that improve the efficiency of Monte Carlo. I have contributed to a novel and extremely efficient way of using Monte Carlo during an accident scenario, and I am currently working to incorporate thermal hydraulics into this numerical scheme.

Logan Kunka (logankunka@tamu.edu)
Degree in Progress: PhD, Aerospace Engineering, Texas A&M University ✦ **Advisor**: Dr. Elaine Oran ✦ **CSGF**: 2018-Present

Research Topic

Reactive fluid physics

Research Responsibilities

During my practicum at Los Alamos National Laboratory (LANL), I developed detailed chemical kinetics models for reacting flows. This entailed using physics-based simulations and continuum models for fluids that were undergoing sometimes both chemical reactions and phase changes. Understanding the behavior of materials as they experience these processes helps provide information about the deflagration and detonation properties of reactive material as well as transitions between states.

One of the highlights of my time at LANL was seeing the breadth of problems that the lab solves. Scientists and engineers who are leaders in their field and passionate about tackling hard problems support these efforts. The ability to quickly chat with these experts about their research or the problems I face in my own research was a unique experience I doubt I would find in other places. The historic significance and the generations of experience at LANL makes it a very exciting place to work.

Benefits of CSGF

I believe the DOE CSGF community is a large part of what makes the program great. The network of fellows and alumni is incredibly active. It's not uncommon to encounter other fellows at conferences or alumni in positions in industry and academia or at the national laboratories.

The annual review gives us the opportunity to network and understand the science other fellows pursue. Participants can see how computational science is used in other fields and often start research collaborations with those of similar interests. Computational science is an extremely broad field, and the variety of topics presented at the program review reflect that.

One large benefit the DOE CSGF program provided was the research freedom to pursue challenges that interested me. This extends both into academic research as well as the practicum, where fellows can experience the national laboratory culture and gain exposure to or learn skills in areas that typically are outside their graduate program. I encourage anyone interested in computational science to apply.

Alicia Magann (abmagann@gmail.com)

Degree: PhD, Quantum Control, Princeton University ✦ **Advisor**: Dr. Herschel Rabitz ✦ **CSGF**: 2016-Present

Research Topic

Quantum information science

Research Responsibilities

Through the Department of Energy/National Nuclear Security Administration (DOE/NNSA) CSGF program, I spent two summers doing quantum information science research at Sandia National Laboratories (SNL). I first worked with Matthew Grace, Mohan Sarovar, and my PhD advisor, Herschel Rabitz, to develop a hybrid algorithm that uses both quantum and classical computers in tandem to compute pulses to control molecular dynamics. The project produced a manuscript and introduced me to quantum information science in the context of its application toward coherent control of molecules using lasers. Although I was familiar with the application, quantum information science was something new and exciting to me.

I returned to SNL the following summer, this time studying a different quantum computing application: optimization. With Matthew, Mohan, and Kenneth Rudinger, I worked to develop a quantum algorithm to identify approximate solutions to combinatorial optimization problems inspired by ideas from Lyapunov control theory. We are preparing a manuscript and hope our approach will have applications in the noisy, intermediate-scale, quantum era.

Perhaps the most important highlight of my SNL experience was the chance it provided to see what a National Nuclear Security Administration laboratory career looks like. I realized this could be a great fit for me, one that I otherwise might not have considered. Another highlight was meeting and engaging with so many outstanding researchers working on aspects of quantum information science, which has given me a sense of the diverse research SNL pursues in this area.

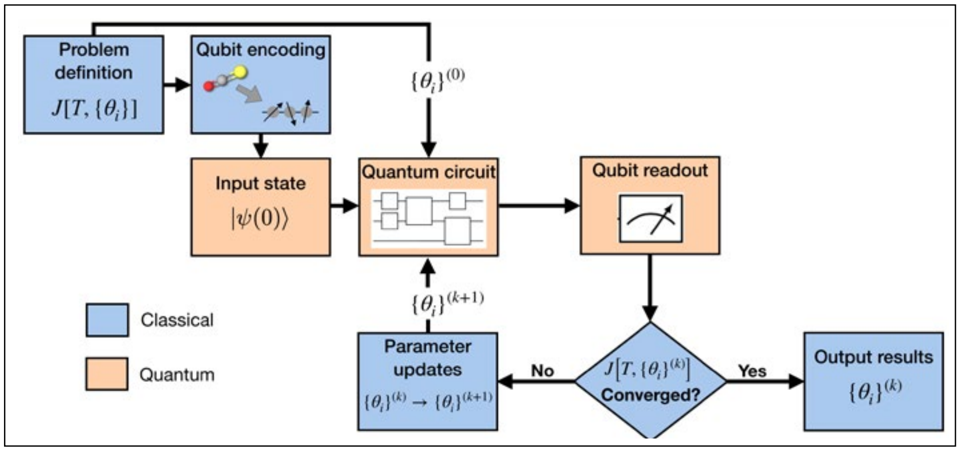


Figure 1. Block diagram of hybrid quantum-classical algorithm for designing parameterized laser fields to control molecular dynamics.

"Perhaps the most important highlight of my SNL experience was the chance it provided to see what a National Nuclear Security Administration laboratory career looks like. I realized this could be a great fit for me, one that I otherwise might not have considered. Another highlight was meeting and engaging with so many outstanding researchers working on aspects of quantum information science, which has given me a sense of the diverse research SNL pursues in this area."

Benefits of CSGF

The CSGF has had a significant impact on my PhD experience. Broadly speaking, it has given me more independence in research, which is something I've come to value tremendously. I've had more freedom to think of and pursue new ideas.

The practicum component, and my experiences at SNL, have also tangibly affected my research by introducing me to quantum information science and redirecting the latter half of my PhD to include not only the coherent control of molecules, but also applications of quantum computing. This would have been impossible without the CSGF.

These experiences have influenced my career goals. The caliber of research at SNL and at the other DOE national laboratories so impressed me that they've become my top choice when it comes to pursuing postdoctoral positions and fellowships.

Amy Lovell, Los Alamos National Laboratory (lovell@lanl.gov)
Years at LANL: 2018-Present ✦ **Degree:** PhD, Physics ✦ **SSGF:** 2015-2018, Michigan State University

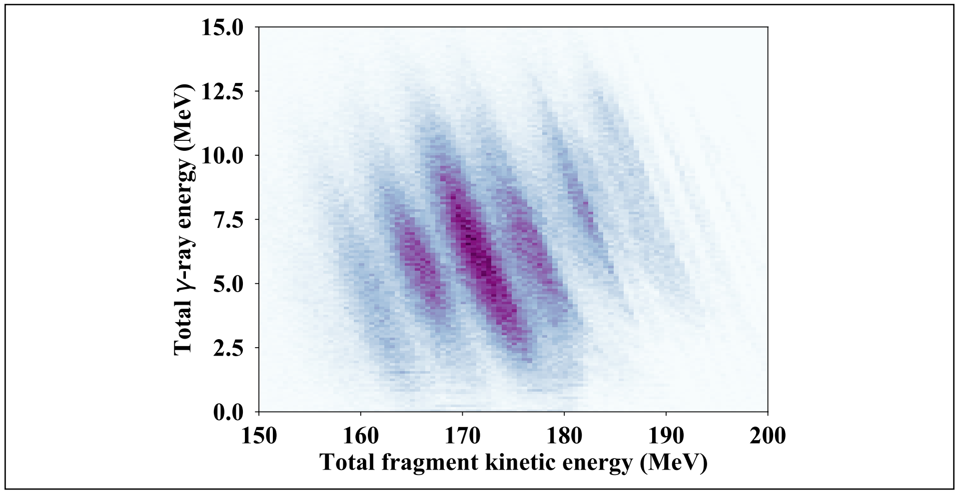


Figure 1. Calculated correlations between fission fragment kinetic energies and total γ-ray energy emitted by the fission fragments.

I was a graduate student at Michigan State University, having my first real opportunity to conduct research in theoretical nuclear physics at the National Superconducting Cyclotron Laboratory (NSCL) when I was encouraged to apply for the Stewardship Science Graduate Fellowship. At the time, I had been studying exotic, three-body nuclei—nuclei with an unusually large number of protons or neutrons that can be approximated as three particles instead of as an A-body system—and my thesis advisor, Professor Filomena Nunes, had been interested in investigating uncertainties in reaction theory in a well-quantified manner. I decided to pursue uncertainty quantification for my thesis topic, focusing on parametric uncertainties in the phenomenological potentials used to describe few-body nuclear reactions.

When I found out that I had been chosen as an Stewardship Science Graduate Fellowship (SSGF) fellow, I had already had a brief introduction into the Stewardship Science Academic Programs, as my thesis adviser was part of a Stockpile Stewardship Academic Alliances (SSAA) Center for Excellence in nuclear physics. The Stewardship Science Graduate Fellowship broadened and deepened that first introduction, and I greatly benefitted from interacting with the other fellows, both present and past, the laboratory staff, and a wide range of program directors. After being so deeply entrenched in nuclear physics at the NSCL, the SSGF and SSAA program reviews gave me a better understanding of the NNSA laboratory missions and the breadth of science in which they are interested. In addition, I gained a network outside of nuclear physics.

While my group at the NSCL had collaborators at Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory, the SSGF practicum gave me the opportunity to work on a project outside of reaction theory. I did my practicum at LANL, working on an uncertainty quantification project to examine model features for hydrocarbons diffusing through shale. The project was a far cry from nuclear physics, but it allowed me to explore a variety of uncertainty quantification techniques that were being used at LANL. During my practicum, I remained connected to the nuclear theory group at LANL which directly led to my postdoctoral position.

"... I greatly benefitted from interacting with the other fellows, both present and past, the laboratory staff, and a wide range of program directors. After being so deeply entrenched in nuclear physics at the NSCL, the SSGF and SSAA program reviews gave me a better understanding of the NNSA laboratory missions and the breadth of science in which they are interested."

After a successful dive into hydrology during my practicum, I decided to change my focus slightly for my postdoc. I joined the nuclear theory group at LANL to study fission theory, investigating the correlations between the fission fragments and emitted neutrons and γ rays, as in Figure 1 which shows correlations between the fission fragment and γ-ray energies. To study these correlations, we consistently model a part of the fission process, beginning with the initial conditions of the fission fragments through the evaporation of the prompt neutrons and γ rays, including conservation of energy, spin, and parity at each step in the decay in a Monte Carlo fashion. The full history of each event is recorded, and we can reconstruct average and correlated quantities. Our close collaboration with experimentalist at LANL allows us to compare our predictions with their measurements.

At the end of 2019, I was converted to a staff scientist position in the theory group at LANL. I am continuing to study correlations in fission observables and am again broadening my knowledge. In addition to the correlated fission work, I have begun to work on nuclear data evaluations, combining experiment and theory to provide recommended values to the community, including realistic uncertainties. I am grateful for the opportunities that the SSGF provided, leading to my current position, and look forward to building upon those opportunities as my career continues.

Sylvia Hanna (sylviahanna2022@u.northwestern.edu)
Degree in Progress: PhD, Chemistry, Northwestern University ✦ **Advisor**: Dr. Omar K. Farha ✦ **SSGF**: 2019-Present

Research Topic

Actinide-based metal–organic frameworks

Research Responsibilities

My research revolves around designing and synthesizing uranium-based metal–organic frameworks (MOFs). MOFs are porous, crystalline materials that remarkably self-assemble from inorganic nodes and organic linkers into beautiful nets that extend in two, or three, dimensions. Most research in the field of MOFs has been performed on frameworks based on lighter-metals, such as transition metals. Whereas some design rules for lighter metal MOFs can be extended to actinide-based MOFs, actinides have inherent chemical differences due to the presence of f-electrons. My research focuses on developing design rules and structure-property relationships for actinide MOFs, specifically uranium-based MOFs. I primarily employ solvothermal synthesis, crystallography, and gas physisorption to determine the underlying design principles that make uranium-based MOFs different from lighter-metal MOFs. My research has underlying applications and use in 1) uncovering unique electronic and bonding behavior of uranium by placing it into frameworks with novel coordination chemistry and 2) developing actinide-based MOFs for nuclear-fuel-industry-related applications and nuclear waste disposal. Drawing from my interest in actinides, I also study the effect of ionizing radiation, such as gamma rays, on MOFs. Determining if MOFs are stable under these extreme conditions is vital before using MOFs for applications such as radionuclide capture and nuclear waste disposal.

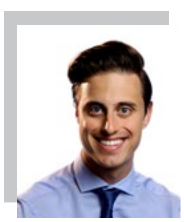
Benefits of SSGF

The SSGF fellows are a unique group of highly intelligent, skilled scientists who are also personable and approachable. Being welcomed into this group of students has granted me an immediate community that I am deeply appreciative of. The SSGF Program has given me the opportunity to interact with scientific expertise outside of my immediate field of study, which is incredibly valuable. Finally, I have been able to learn an enormous amount about the national laboratories and stewardship science through the SSGF.

National Laboratory Experience

If you are unsure if your research fits into the SSGF umbrella, apply anyway. There is such a broad range of scientific questions and expertise related to the National Nuclear Security Administration that is funded by this fellowship. Additionally, this means that you will have a plethora of exciting scientific projects to learn about and become exposed to that you would not have had the chance to otherwise.

Chad Ummel (chadummel@physics.rutgers.edu)
Degree in Progress: PhD, Physics, Rutgers University ✦ **Advisor:** Dr. Jolie Cizewski ✦ **SSGF**: 2018-Present



Research Topic

Measuring the $^{134}Te(d,p\gamma)^{135}Te$ Reaction with GODDESS to Probe the Single-Particle Structure of ^{135}Te

Research Responsibilities

^{135}Te has been identified as an important isotope for both nuclear structure studies and nuclear astrophysics—for the latter, specifically in attempts to explain an overabundance of ^{134,136}Xe observed in some pre-solar meteorite grains. The single-neutron structure of ^{135}Te can be constrained using neutron-transfer reactions such as (d,p) in coincidence with the detection of gamma rays emitted by its excited states. To this end, I participated in a measurement of the ^{134}Te(d,pγ)^{135}Te reaction with the GRETINA-ORRUBA: Dual Detectors for Experimental Structure Studies (GODDESS) detection system at Argonne National Laboratory (ANL), and I am leading the analysis of the data collected. I am a core member of the GODDESS and Oak Ridge Rutgers University Barrel Array (ORRUBA) collaborations, and I participate in a number of experiments at both ANL and the National Superconducting Cyclotron Laboratory performing similar measurements on nuclei that are important for stockpile stewardship and nuclear astrophysics.

Benefits of SSGF

SSGF has provided me with unparalleled support which has allowed me to focus completely on my research. The annual program reviews have been a fantastic opportunity to network. I have enjoyed meeting SSGF alumni and learning about opportunities after graduate school (including many that I had never before considered). I also have enjoyed touring the national laboratories and learning about the stewardship work being done at those locations.

National Laboratory Experience

The national laboratories have been pivotal to my growth as a scientist. I got my start in research as a summer undergraduate intern with Sandia National Laboratories-California in 2014. Following that, I joined a research group at UC Berkeley and participated in a number of experiments at Lawrence Berkeley National Laboratory over the following two years. I completed another summer internship at Sandia National Laboratories-New Mexico in 2015. As a member of the GODDESS and ORRUBA collaborations, I spend nearly 100% of my time in residence at Oak Ridge National Laboratory working with my collaborators to prepare for experiments (three of which were performed at ANL).

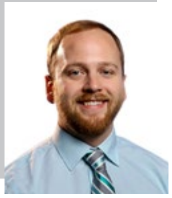
SSGF also gave me the opportunity to spend the Fall of 2019 completing a practicum at Los Alamos National Laboratory. During my time at LANL, I led the development of a Geant4 simulation package for the Detector for Advanced Neutron Capture Experiments (DANCE) at the Los Alamos Neutron Science Center. It was rewarding to see my work directly benefit the DANCE research program and I am incredibly grateful that SSGF provided me with this opportunity.

Dane Sterbentz (dmsterbentz@ucdavis.edu)

Degree in Progress: PhD, Mechanical and Aerospace Engineering, University of California, Davis ✦ **Advisor:** Dr. Jean-Pierre Delplanque ✦ **LRGF:** 2019-Present

Research Topic

Numerical Modeling of the Sub-microsecond Solidification of Materials undergoing Dynamic Compression



Research Responsibilities

My research involves modeling the sub-microsecond phase transition kinetics of materials in dynamic-compression experiments using methods based in classical nucleation theory (CNT). These types of dynamic-compression experiments are used to investigate the behavior of materials under extreme pressures. The main focus of my research is on the solidification of liquid water to the ice VII phase (a high-pressure, solid-water polymorph). I have conducted an investigation of the transient behavior of the solidification kinetics using a fundamental CNT-based kinetics equation. I have developed a novel method for determining the drive pressure in ramp-wave compression experiments using a heuristic optimization algorithm, which is an essential part of conducting multiscale simulations of these experiments. One phenomenon for which a theoretical explanation still is missing, despite the fact that it has been observed in experiments for decades, is the variation between experiments in the lag time that occurs after crossing the phase boundary and before the transition actually occurs. I am attempting to provide a mechanistic understanding of this lag time by investigating the compression-rate dependence of the phase transition kinetics in these experiments.

Benefits of LRGF

The LRGF program has given me the financial freedom to focus full-time on my research as well as the opportunity to work closely with world-class researchers on a series of exciting and cutting-edge topics. The NNSA laboratory residency aspect of the LRGF program has been a particularly great opportunity, as it has allowed me to work on-site and has provided an inside look at what a career at a NNSA national laboratory might be like. The LRGF program also has provided me with the opportunity to network with researchers in the field of stewardship science from a number of other NNSA laboratories and academic institutions and learn about fascinating innovative and emerging research topics.

National Laboratory Experience

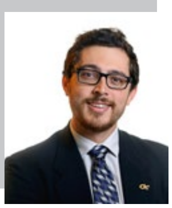
My experiences while conducting the NNSA laboratory residencies have convinced me that working at a national laboratory is one of the best possible career paths available to young researchers. Working on-site at a national laboratory not only has provided me with the unique tools needed to complete my research but has provided me with the opportunity to gain a broader perspective on and greater appreciation for the scope and importance of the diverse research conducted at a national laboratory.

Travis J. Voorhees (tjvoorh@sandia.gov, tjvoorhees@gatech.edu)

Degree in Progress: PhD, Materials Science and Engineering, Georgia Institute of Technology ✦ **Advisor:** Dr. Naresh N. Thadhani ✦ **LRGF:** 2018-Present

Research Topic

High-Precision Measurements and Modeling of How Brittle Granular Materials Behave under Shock Compression



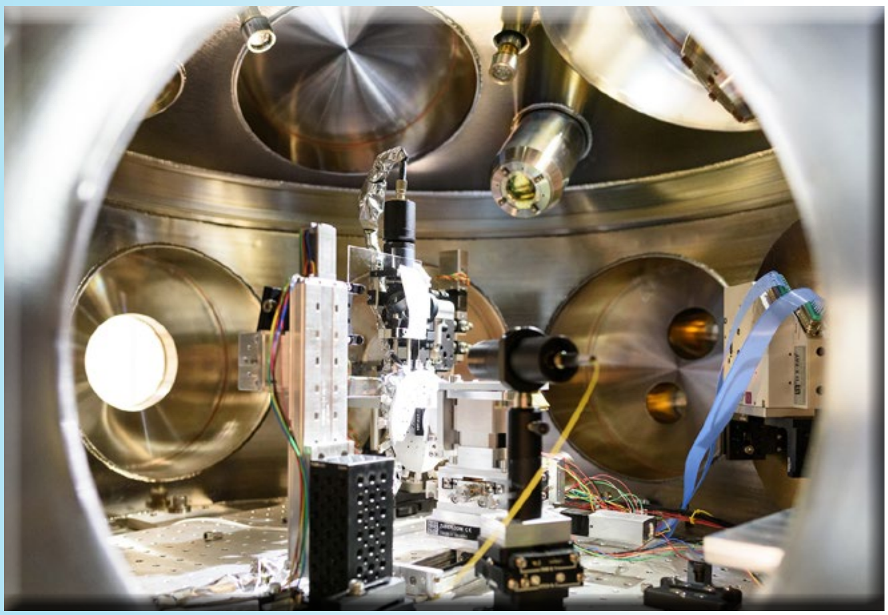
Research Responsibilities

I spend two-thirds of my time at the Georgia Institute of Technology (Georgia Tech) and one-third at Los Alamos National Laboratory (LANL). At Georgia Tech, I design, create, execute, and analyze high-precision, plate impact experiments on CeO_2 powder. I design my projectiles and targets using CAD software, then hand-machine these high tolerance parts using a lathe, mill, and various hand tools. I execute the experiments using an 80 mm light gas gun. To accurately measure the compaction response of the CeO_2 powder, I designed and built a 24-measurement, multiplexed photonic Doppler velocimetry (MPDV) system. To robustly analyze the MPDV signals measured during impact experiments, I created a high-fidelity analysis code, HiFiPDV, that calculates the most likely velocity-time history from the MPDV intensity-time signal and its corresponding time-dependent velocity uncertainty. Using the velocity measurements from the impact experiments, I calculate how CeO_2 powder responds to shock compression as a function of initial state (initial density, etc.) and shock compression pressure.

At LANL, I use the high-performance computing systems (HPC) to design complex-geometry shock compression experiments on CeO_2 powder, then execute the experiments at the LANL proton radiography (pRad) facility using the pulsed power driver PHELIX. I use the pressure-density data gathered during my Georgia Tech impact experiments to calibrate computational models for the compaction response of CeO_2 powder. Using the LANL code FLAG, I simulate the complex-geometry experiments, capturing both the magnetohydrodynamic behavior of PHELIX and the mechanical response of the CeO_2 powder. Working with the LANL pRad and PHELIX teams, we executed two pulsed power shock compaction experiments on CeO_2 powder. The proton radiographs collected from these experiments have helped me generate and validate computational models for how CeO_2 powder, and other brittle granular materials, will respond to shock compression in a variety of geometries.

Benefits of LRGF

The community that I have become a part of by joining the LRGF program is invaluable. I truly enjoy spending time with the other SSGF and LRGF fellows and alumni. They have helped me gain a deeper understanding of complex physics, been travel partners in residency and program review locations, and have been a huge support in all areas of graduate school life. These fellows are the people with whom I plan to collaborate and work throughout my scientific career.



User Facilities

Dynamic Compression of Materials: Real-Time Multi-Scale Measurements

Washington State University ✦ PI: Dr. Y.M. Gupta (ymgupta@wsu.edu)

Background

Since the pioneering developments over 70 years ago at Los Alamos National Laboratory, shock wave (or dynamic compression) experiments have played a seminal role in studying materials' response at the most extreme thermophysical conditions involving pressure, temperature, and deformation. A unique feature of shock experiments is the ability to examine material response in real-time (ps-µs)—essential for understanding and modeling fundamental mechanisms. Past experiments have focused primarily on thermodynamic results, and the need for augmenting these with measurements at lower length scales—atomic/micro/meso scales—has long been recognized as central to scientific frontiers in diverse disciplines, national security applications, and technology advances.

The Dynamic Compression Sector (DCS), a national user facility located at the Advanced Photon Source (APS) and operated by Washington State University, was established by the Department of Energy (DOE)/National Nuclear Security Administration (NNSA) to address the key need regarding real-time, multiscale measurements. This first-of-its-kind experimental capability (worldwide) has linked state-of-the-art, dynamic compression platforms with the bright, high energy, X-ray beam at the APS to achieve the desired measurements under high stress impulsive loading—stresses to 500 gigapascal and durations from 5 nanoseconds to a microsecond. Since 2018, the four experimental stations (Impact Facilities (Figure 1), Laser-Shock, and Special Purpose) have been fully operational – utilizing time-resolved X-ray (diffraction, phase contrast imaging, and scattering) and continuum (laser interferometry) measurements. A wide range of user experiments have successfully addressed long-standing scientific challenges. Visit dcs-aps.wsu.edu for details regarding DCS capabilities, publications (2016-present), and guidance for user experiments.

Recent Enhancements

In the past year, new capabilities were incorporated in the Laser-Shock Station. One is Extended X-ray Absorption Fine Structure (EXAFS) measurements—complimentary to X-ray Diffraction (XRD)—to probe local, atomic structure in crystalline, non-crystalline, and disordered materials (Rev. Sci. Instr. 91, 085115, 2020). A second is a line-VISAR for high spatial resolution measurements. Another is highly reproducible, uniform compression over 1 mm diameter—augmenting the current 500 µm diameter capability—resulting in a broader range of stresses and sample sizes.

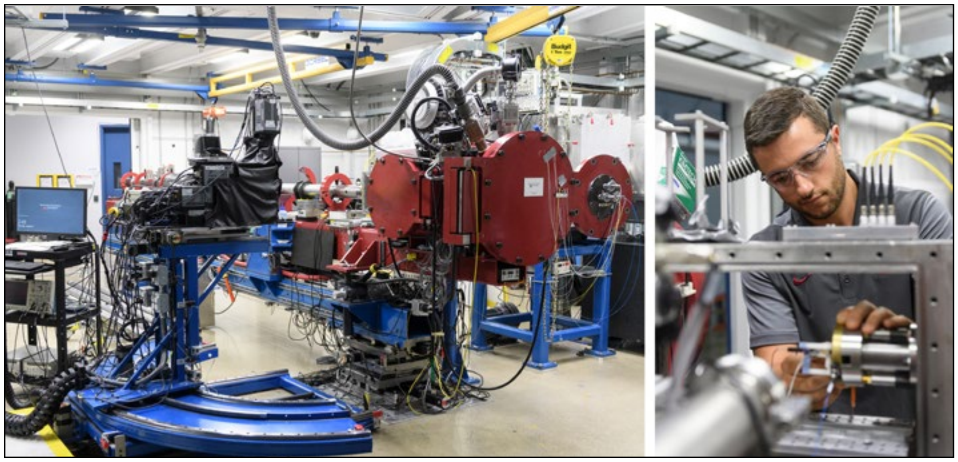


Figure 1. Impact Facilities: Two-stage gun and X-ray detectors (left) and mounting a target (right).

APS Upgrade

Between Spring 2022 and Summer 2023, the APS synchrotron will undergo a major upgrade to produce X-rays having higher brilliance and coherence (aps.anl.gov/APS-Upgrade). Reduction in separation between X-ray pulses from 154 ns to 77 ns will provide improved insight into time-dependent phenomena. Higher brilliance and beam coherence will expand significantly the scientific opportunities by permitting measurements not currently available. To maximize the upgraded beam benefits for user experiments, the DCS will undertake complementary upgrade activities to continue as the premier user facility for addressing future scientific challenges. Planned upgrades include new undulators, advanced X-ray optics, state-of-the-art X-ray diagnostics, and enhancements to dynamic compression platforms.

General User Experiments

Training the next generation of scientists to address fundamental challenges—by utilizing the DCS capabilities—is an important goal of the DCS General User (GU) program, emphasizing academic users. Visit dcs-aps.wsu.edu/proposal-submission for information regarding GU proposal submission. Examples of academic research activities made possible by the DCS capabilities are summarized below.

Scientific Highlights (Academic Users)

Shock Compression of Quartz (Sci. Adv. 6: eabb3913, 2020)

Despite extensive research spanning five decades, key issues regarding structural transformations in shock-compressed quartz have remained unresolved. XRD measurements provide direct evidence that quartz transforms to a disordered high pressure phase as opposed to crystalline stishovite or an amorphous structure, challenging longstanding assumptions.

Shock Induced Formation of Cubic and Hexagonal Diamond (Phys. Rev. B. 101, 224109, 2020)

Shock compression experiments on different types of graphite have reported hexagonal diamond and cubic diamond formation at comparable stresses. XRD measurements have resolved these disparate findings by demonstrating that the diamond structure formed is governed by the initial graphite structure and microstructure.

FCC-BCC Transformation in Shock Compressed Noble Metals (Phys. Rev. Lett. 124, 235701, 2020)

XRD measurements provided the first observations of the fcc-bcc transformation in shock-compressed gold and silver (subsequently, in copper) but not in platinum. The occurrence of this unexpected structural change was linked to stacking faults produced under shock compression.

Travis Volz , Lawrence Livermore National Laboratory (volz2@llnl.gov)
Years at LLNL: April 2020-Present ✦ **Degree:** PhD, Physics ✦ Years in Academic Programs: 2014-2020, Washington State University

I first became involved with the Stewardship Science Academic Programs (SSAP) and the exciting field of dynamic compression science while pursuing my PhD at the Institute for Shock Physics (ISP) at Washington State University. My PhD research, completed under the guidance of Professor Yogendra Gupta, focused on understanding shock-wave-induced phase transformations: specifically, the role of different graphite crystal structures and microstructures on the shock-induced graphite to diamond phase transformation. My research utilized two world-class experimental capabilities funded by the Department of Energy/National Nuclear Security Administration (DOE/NNSA): the ISP, and the Dynamic Compression Sector (DCS).

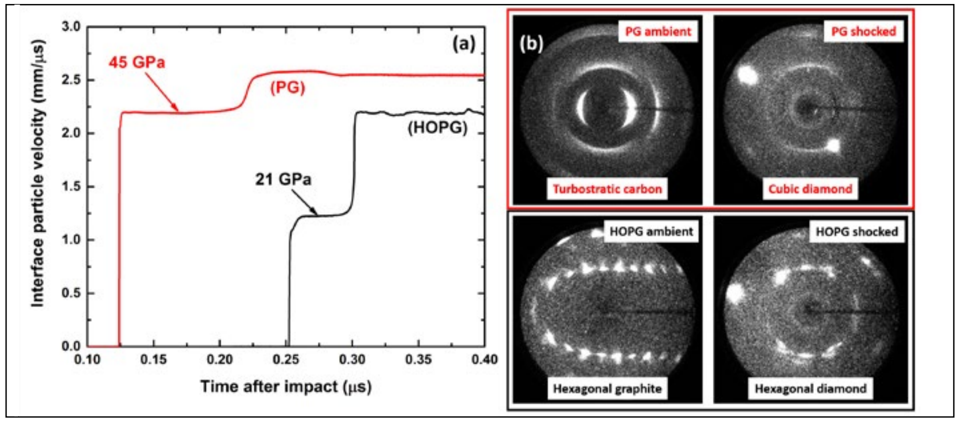


Figure 1. (a) Wave profiles and (b) XRD images from PG (red) and HOPG (black). Transformation stresses are labeled in (a), and the ambient and high-stress crystal structures are labeled in (b). Data in (a) and (b) are from Volz et al., J. Appl. Phys. 125, 245902 (2019), and Volz et al., Phys. Rev. B 101, 224109 (2020), respectively.

At the ISP, I learned how to conduct shock experiments and used laser interferometry to quantify the shock compression responses of several graphite types. By analyzing the measured wave profiles (Figure 1a), I determined the stresses required to transform each graphite type to its high-stress phase. The transformation stress for the as-deposited pyrolytic graphite (PG) was more than double that of the highly-oriented pyrolytic graphite (HOPG). To better understand the mechanisms responsible for the different continuum responses and to determine the high-stress crystal structures in shock-compressed graphite, I performed *in-situ* X-ray diffraction (XRD) experiments at the DCS. My work showed that HOPG transforms to the rare hexagonal diamond structure under shock compression. In contrast, crystallographic disorder in the PG facilitates transformation to the more common cubic diamond structure. Hands-on experience at two unique experimental facilities, ISP and DCS, was invaluable for completing my PhD research and for my learning to be an independent researcher.

Throughout my PhD research, I was fortunate to interact with scientists from the DOE/NNSA laboratories during their visits to the ISP (for reviews and seminars) and through my attendance at the SSAP Annual Symposia. These interactions exposed me to a broad range of exciting dynamic compression research occurring at the NNSA laboratories and piqued my interest in pursuing a career there. This interest was strengthened while doing experiments at the DCS where I collaborated with shock physicists and X-ray scientists in a fast-paced, research environment. The connections I made throughout my PhD studies and my desire to continue dynamic compression research in collaboration with outstanding scientists working at the most advanced experimental facilities, ultimately led to my current postdoctoral (postdoc) position at Lawrence Livermore National Laboratory (LLNL).

During my postdoc, I have been able to apply both of my dynamic compression continuum scale and XRD backgrounds to LLNL's scientific and programmatic missions. One project I am working on at LLNL uses the National Ignition Facility (NIF) to gradually ramp compress samples to study their behavior at some of the most extreme conditions in the solar system (pressures comparable to those at the cores of planets). At a given pressure, ramp compression results in considerably lower temperatures than shock compression. This allows us to study solids at very high densities and pressures. We can even quantify the strength of the solid phase at these conditions. Measuring strength is a very recent and exciting development for the NIF ramp compression platform and is central to obtaining an accurate understanding of materials at extreme conditions.

Another project I am working on at LLNL applies XRD techniques to better understand how crystal structures and material microstructures evolve during shock compression. My work involves using forward XRD simulations to understand how small crystallites within a larger sample are re-oriented and change structures during shock compression. This information provides key insight into the underlying microscopic processes occurring during shock compression. Unparalleled access to world-class, experimental capabilities and scientists with a diverse range of backgrounds is a major benefit of working at an NNSA laboratory—a benefit I have experienced firsthand, even though I have been at LLNL less than one year.

"...I was fortunate to interact with scientists from the DOE/NNSA laboratories during their visits to the ISP (for reviews and seminars) and through my attendance at the SSAP Annual Symposia. These interactions exposed me to a broad range of exciting dynamic compression research occurring at the NNSA laboratories and piqued my interest in pursuing a career there."

High Pressure Collaborative Access Team—A Dedicated Facility for Studying Materials at Extreme Pressure and Temperature

Advanced Photon Source, Argonne National Laboratory ✦ Authors: Dr. Nenad Velisavljevic (HPCAT-Director@anl.gov) and Dr. Maddury Somayazulu (zulu@anl.gov)

Located at the Advanced Photon Source (APS) on the campus of Argonne National Laboratory (ANL), the High Pressure Collaborative Access Team (HPCAT) is a dedicated facility for experimental research on materials under extreme pressure-temperature (P-T) conditions. With the strong support from the National Nuclear Security Administration (NNSA), the NNSA national laboratories, the Department of Energy's Office of Science (DOE-SC), and academia, HPCAT was established in the early 2000s concurrent with the formation of NNSA. HPCAT is managed in a collaboration between Lawrence Livermore National Laboratory (LLNL) and APS and fully funded by NNSA.

The primary experimental focus at HPCAT is on research and development of synchrotron X-ray techniques and coupling these with diamond anvil cell (DAC) and large volume press (LVP), P-T platforms (Figure 1).

With four, simultaneously-operational, experimental beamline stations, our users are provided X-ray experimental probes, covering an array of diffraction, imaging, and spectroscopy techniques (additional information is available on HPCAT website at https://hpcat.aps.anl.gov/).

Scientific Highlights

Our experimental capabilities are used to obtain critical and fundamental data in support of stewardship science and, more broadly, to advance the scientific study of matter under extreme P-T conditions. With the Dynamic Compression Sector (DCS), an NNSA-funded facility at APS-ANL and operated by Washington State University that came online in 2018, the NNSA user community now has access to a wide assortment of experimental capabilities for X-ray measurements covering a range of P-T and strain rate conditions. Recently, X-ray measurement capabilities were used by NNSA laboratory partner-users to examine structural phase stability in zirconium[1] and cerium[2] under dynamic and DAC compression (Figure 2). In a separate set of experiments, using laser heating and the DAC capability at HPCAT, an NNSA laboratory postdoctoral fellow user further extended the measurement of the P-T phase stability of zirconium across the solid-melt boundary.[3] These measurements provide critical P-T data for the development of multi-phase equation-of-state models, supporting hydrodynamic code development, and other NNSA mission-relevant work. Each year HPCAT contributes to 100+ peer reviewed journal publications and supports numerous milestone efforts by NNSA laboratories.

Figure 1. Various diamond anvil cell (DAC) platforms available and used for high- pressure experiments at HPCAT.

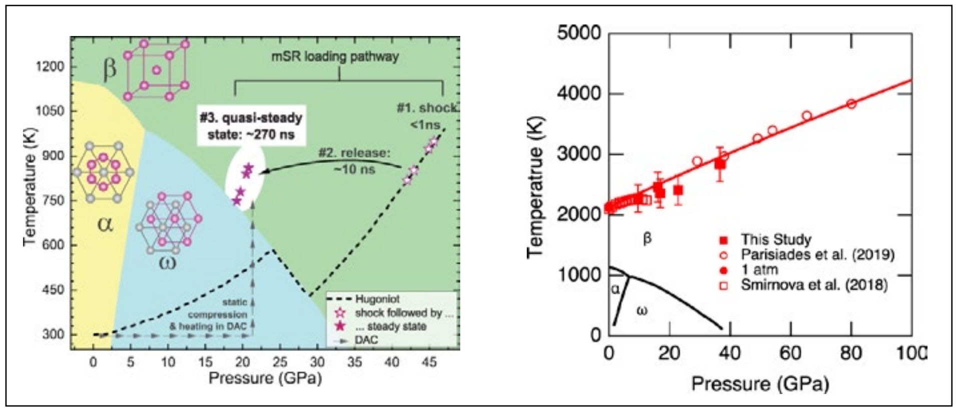


Figure 2.Left: P-T phase diagram and structural phase stability in zirconium studied using shock and DAC compression techniques and X-ray measurements at HPCAT and DCS.[1] Right: High pressure melt boundary of zirconium.[3]

Figure 3. HPCAT student users at the February 2020 SSAP symposium in Washington, DC. Left: Kaleb Burrage, PhD student with Professor Y. K. Vohra at the University of Alabama at Birmingham and graduate student researcher at Sandia National Laboratories, discussing some of the recent work done using University of Alabama at Birmingham's designer diamond anvils and measurements at HPCAT with Dr. William Bookless, Principal Deputy Administrator of NNSA. Right: Benjamin Brugman, PhD student with Professor S. Dorfman at Michigan State University, Outstanding Poster Award winner, discussing Strength, Deformation and Equation of State of Tungsten Carbide to 66 GPa experimental work performed at HPCAT.

User Community

As the largest, dedicated, high-pressure, synchrotron-based user facility in the world, HPCAT hosts over 800 users per

Figure 4. Various workshops, training, and recruitment events are organized by HPCAT. From the January 2020 “Introduction to Technique and Capabilities at HPCAT” workshop - Left: Professor Avinash Dongare University of Connecticut from the SSAA Center for Research Excellence on Dynamically Deformed Solids and Middle: Students and HPCAT interact during one of the training/demonstration sessions. Right: Chicagoland High School students getting a chance to perform some high-pressure experiments at HPCAT.

year: partner-user NNSA laboratories, Stockpile Stewardship Academic Alliance (SSAA) partners (75%) and a broader high pressure, scientific, general-user community (25%). Students and postdoctoral researchers make up about 50% of all the user base (Figure 3). Over the course of the 2019-2020 graduation period, 19 PhD degrees were granted to HPCAT student users, with at least nine continuing work as postdoctoral fellows or research staff at national laboratories.

Student and next-generation staff training is vital, and in addition to maintaining cutting edge X-ray and high P-T capabilities, a significant portion of HPCAT staff’s effort is dedicated to recruitment, training, and expanding our user community. In January of 2020, HPCAT organized and hosted a workshop that was focused on new users, mostly out of the SSAA program and other early career researchers from the high-pressure community. With over 50 participants in attendance, the workshop was a great opportunity for building collaborations and for HPCAT to demonstrate the experimental capabilities with hands on training (Figure 4). HPCAT co-hosts a monthly High-Pressure Interest Group seminar that brings together researchers to discuss advancement of high-pressure science. In addition to focusing on some of the high-pressure career researchers, HPCAT has partnered with APS-ANL in supporting other outreach program efforts. During the past academic school year, HPCAT staff hosted several Chicagoland high school students. These students were introduced to various aspects of synchrotron-based research and the many exciting opportunities in science, technology, engineering, and mathematics (Figure 4). Our work with local schools demonstrates both HPCAT and NNSA’s commitment to fostering next-generation scientists and actively participating in community stewardship.

References

[1]P. Kalita, J. Brown, P. Specht, S. Root, M. White, and J.S. Smith, PRB 102, 060101(R) (2020).

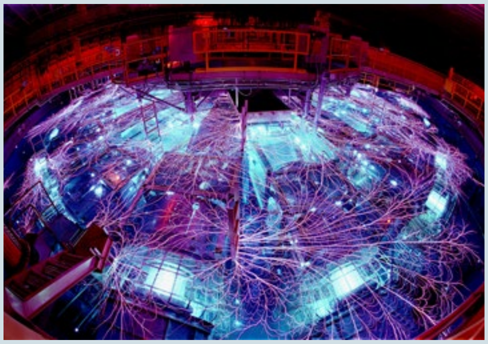
[2]B. Jensen, F. Cherne, and N. Velisavljevic JAP 127, 095901 (2020).

[3]J. Pigott, N. Velisavljevic, E. Moss, N. Draganic, M. Jacobsen, Y. Meng, R. Hrubiak, B. Sturtevant, J. Phys.: Cond.. Matter 32, 355402 (2020).

Dynamic Integrated Compression Experimental Facility

The Dynamic Integrated Compression Experimental (DICE) facility at Sandia National Laboratories is one of few experimental test facilities in the world that can provide multiple platforms for material property study utilizing compressed gas launchers and ramp-loading pulsers with pulse shaping abilities. Unique to DICE is the ability to perform not only shock, or isotropic, compression but also ramped, or isentropic, compression of materials. This allows direct comparison under different distinct loading conditions of the sample under test. A typical DICE gas gun shot consists of a projectile with an impactor on the front surface being launched, by compressed gas, down the gun barrel into a target sample. For more information visit http://www.sandia.gov/Pulsed-Power/research_facilities/index.html. Interested users may contact Gordon Leifeste (gtleife@sandia.gov).

Z Pulsed Power Facility



The Z Pulsed Power Facility (Z) is a megajoule-class pulsed power accelerator and multifaceted experimental resource at Sandia National Laboratories that produces intense X-rays and magnetic fields useful for experiments in fundamental high-energy-density (HED) science. Approximately 10% of the Z shots allocated—around 14 shots/year—are designated for the Z Fundamental Science Program. These shots are competitively awarded to academic, industrial, and national laboratory research interests through a yearly proposal process for state-of-the-art fundamental research in HED physics, including hydrodynamics, properties of materials under extreme conditions, laboratory astrophysics, advanced ignition concepts, fundamental HED physics, biology, and chemistry. The Call for Proposals is typically issued in mid-June and closes in mid-September. The Z Fundamental Science Workshop is held in early August. Award notifications are provided in mid-December for a two-year award period that begins the following July. For more information, visit http://www.sandia.gov/Pulsed-Power/workshop/2020.html or contact Marcus Knudson, mdknuds@sandia.gov.

Shock Thermodynamic Applied Research

The Shock Thermodynamic Applied Research (STAR) facility at Sandia National Laboratories is specifically designed, staffed, and used by professionals in the technical disciplines of High Temperature/High Pressure Condensed Matter Physics, Shock Physics, and Dynamic Material Properties. It is the only experimental test facility in the world that can cover the full range of pressure (bars to multi-Mbar) for material property study utilizing gas/propellant launchers, ramp-loading pulsers, and ballistic applications. STAR houses a collection of five laboratory test launchers (guns) in four gun bays for Dynamic Material Property studies and a small machine shop. For more information visit http://www.sandia.gov/Pulsed-Power/research_facilities/index.html. Interested users can contact Gordon Leifeste (gtleife@sandia.gov).

Omega Laser Facility

The two lasers (EP and OMEGA 60) at the Laboratory for University of Rochester's Laser Energetics (LLE) share over 100 facility-supported diagnostics and perform over 2,300 experiments annually. The staff works closely with the User Community via the Omega Laser Users to add new capabilities every year. Nearly one-third of the experiments on the Omega Laser Facility support basic high energy density science. In fact, three of the past four Dawson awards for Excellence in Plasma Physics Research have relied on data from the Omega Laser Facility. Three programs provide user access (National Laser Users' Facility, Laboratory Basic Science, and LaserNetUSA). Application details are available on the LLE website. For more information, visit www.lle.rochester.edu or contact Dr. Mingsheng Wei, mingsheng@lle.rochester.edu.

The Dynamic Compression Sector

The DOE/NNSA-sponsored Dynamic Compression Sector (DCS) is a first-of-its-kind experimental capability dedicated to understanding the dynamic compression/deformation response of materials through real-time, multiscale measurements. Managed and operated by Washington State University and located at the Advanced Photon Source at Argonne National Laboratory, the DCS uniquely integrates state-of-the-art shock wave and synchrotron x-ray capabilities to provide time-resolved, microscopic measurements under high stress impulsive loading. A wide range of user experiments utilizing X-ray (diffraction, phase contrast imaging, absorption, and scattering) and continuum (laser interferometry) measurements are conducted in each of the experimental stations (Impact Facilities, Laser-Shock, and Special Purpose).For more details and proposal information, visit https://dcs-aps.wsu.edu or contact Dr. Paulo Rigg (dcs.admin@wsu.edu).

The High Pressure Collaborative Access Team

The NNSA-sponsored High Pressure Collaborative Access Team (HPCAT) at sector 16 of the Advanced Photon Source, Argonne National Laboratory, is a synchrotron x-ray facility dedicated for experimental research on materials under extreme pressure-temperature (P-T) and strain rate conditions. The primary experimental focus at HPCAT is on research and development of synchrotron X-ray techniques and coupling these with diamond anvil cell and large volume press, P-T platforms. With four, simultaneously operational, experimental beamline stations, our users are provided X-ray experimental probes, covering an array of diffraction, imaging, and spectroscopy techniques. For more information, visit https://hpcat.aps.anl.gov/ or contact Nenad Velisavljevic (HPCAT-Director@anl.gov). The proposal schedule is as follows: (1) APS: Three operating cycles per year, (2) Experimental time: Obtain via the General User Proposal (GUP) peer reviewed system or internal partner time allocation request, (3) GUP information: https://www.aps.anl.gov/Users-Information/About-Proposals/Proposal-Types/General-User-Proposals, and (4)Partners (including LLNL/LANL/SNL and NNSA-SSAA PIs): Email HPCAT-Director@anl.gov to discuss experimental scope, etc.

Los Alamos Neutron Science Center

For more than 30 years, the Los Alamos Neutron Science Center (LANSCE) has provided the nuclear physics and material science data needed to ensure the safety and surety of the nuclear stockpile. User time is available at the proton radiography (pRad) facility for dynamic radiography, the Lujan Center for neutron scattering and radiography, and the Weapons Neutron Research Facility for nuclear physics. In addition to national security research, LANSCE provides the scientific community with intense sources of neutrons and protons for experiments supporting the production of medical and research isotopes and research in fundamental physics.

Proposal call dates for the various LANSCE experimental areas vary, but they generally open in December/January and run through January/March. For more information, visit https://lansce.lanl.gov or contact Nina Roelofs (nroelofs@lanl.gov).

National Ignition Facility

The National Ignition Facility (NIF) is the world's most energetic laser and is available for user experiments investigating the properties of high-energy-density matter. The NIF provides up to 1.8 MJ of laser energy to targets, with pulse durations that range from sub-ns to 10s of ns. The NIF mail laser can also be coupled to the kJ-class, ps-pulse ARC laser. The NIF's 10-meter-diameter target chamber has multiple lines of sight for optical, X-ray, gamma and neutron, and charged-particle diagnostics. Proposals for user experiments are solicited several times each year. A call for proposals for Discovery Science Users is issued each year. For details, visit https://lasers.llnl.gov/for-users/call-for-proposals and https://lasers.llnl.gov or contact Kevin Fournier, NIF User Office Director, nifuseroffice@llnl.gov.

List of Grants and Cooperative Agreements

Stewardship Science Academic Alliances

High Energy Density Physics

Cornell University
David Hammer
Multi-University Center of Excellence for Pulsed-Power-Driven High Energy Density Science

Massachusetts Institute of Technology
Richard Petrasso
Center for Advanced Nuclear Diagnostics and Platforms for ICF and HED Physics at OMEGA, NIF, and Z

University of California, San Diego
Farhat Beg
Center for Matter Under Extreme Conditions

University of Michigan
Carolyn Kuranz
Center for Laboratory Astrophysics: Structure Formation and Energy Transport After the Dark Ages

University of Texas at Austin
Donald Winget
Center for Astrophysical Plasma Properties

Low Energy Nuclear Science

Duke University
Calvin Howell
Measurements of Short-Lived Fission Product Yields from Photon-Induced Fission of Special Nuclear Materials

Duke University
Werner Tornow
Measurements of Neutron-Induced Fission Product Yields and Fission Neutron Energy Distributions

Michigan State University
Sean Liddick
Neutron Capture Cross Section Measurements on Short-Lived Isotopes

Michigan State University
William Lynch
Asymmetric Nuclear Matter Under Extreme Conditions

Michigan State University
Witold Nazarewicz
Microscopic Description of the Fission Process

Ohio University
Carl Brune
Scattering and Reactions of Light Nuclei

Ohio University
Zach Meisel
Statistical Nuclear Physics and (a,n) Reactions for Applications

Oregon State University
Walter Loveland
The Energy Release in the Fission of Actinide Nuclei

Rutgers University
Jolie Cizewski
Nuclear Reaction Studies with Radioactive Ion Beams for Stewardship Science

Texas A&M University
Sherry Yennello
Center for Excellence in Nuclear Training and University-based Research (CENTAUR)

University of Kentucky
Michael Kovash
Prompt Fission Neutrons from Pu-239

University of New Mexico
Adam Hecht
New Measurements of Independent Fission Fragment Yields and Energies, and Prompt and Delayed Gammas, for Stockpile Stewardship Data Needs

The University of Tennessee, Knoxville
Robert Gryzwacz
Beta-Delayed Neutron Spectroscopy of Exotic Nuclei

Properties of Materials Under Extreme Conditions

Carnegie Mellon University
Robert Suter
Towards Optimal Processing of Additive Manufactured Metals for Applications in Extreme Environments

Georgia Tech Research Corporation
Devesh Ranjan
Detailed Measurements of Turbulent Raleigh-Taylor and Richtmyer-Meshkov Mixing at Extreme Conditions

Harvard University
Stein Jacobsen
From Z to Planets - Phase III

Harvard University
Isaac Silvera
High Pressure Metallic Hydrogen

Johns Hopkins University
Todd Hufnagel
Maximizing Reliability and Information Content of Ramp Compression Experiments with In Situ X-ray Characterization

Research Foundation for the State University of New York
Baosheng Li
Thermodynamic and Mechanical Properties of SSP Materials from Simultaneous Ultrasonic and X-ray Studies at High Pressure and Temperature

Texas A&M University
Michael Demkowicz
Center for Research Excellence on Dynamically Deformed Solids (CREDDS)

University of Alabama at Birmingham
Yogesh Vohra
Studies on Rare Earth Metals and Alloys under Terapascal Pressures in Support of the Stockpile Stewardship Program

University of Arizona
Jeffrey Jacobs
An Experimental Study of Rayleigh-Taylor and Richtmyer-Meshkov Instabilities with Complex Acceleration History

University of Illinois at Chicago
Russell Hemley
Chicago/DOE Alliance Center – A Center of Excellence for High Pressure Science and Technology

University of Nevada, Las Vegas
Pamela Burnley
Deformation of Polycrystalline Materials under Extreme Conditions: Stress Percolation, Shear Localization and Grain Boundary Rheology

University of Rochester
Ranga Dias
Tuning of Competing Quantum States under Extreme Conditions

University of Rochester
Jessica Shang
X-ray Particle Image Velocimetry for HED Science

University of South Florida
Ivan Oleynik
Phase Transitions under Dynamic Compression: Carbon, Silicon, and Germanium

University of Wisconsin, Madison
Riccardo Bonazza
New Experimental Approaches to Study Gas Interfaces Accelerated by Shock Waves

Washington State University
James Hawreliak
Time-Resolved Lattice Kinetics of Rapidly Compressed Single Crystal Iron through the Alpha to Epsilon Phase Transition

Washington State University
C.S. Yoo
Chemistry of Dense Planetary Mixtures at Extreme Conditions

Radiochemistry

Michigan State University
Gregory Severin
Aqueous-Phase Isotope Harvesting to Manufacture Radioactive Targets for Neutron-Reaction Studies

University of Notre Dame
Ani Aprahamian
A Novel Technique for the Production of Robust Actinide Targets

University of Notre Dame
Peter Burns
Actinide Center of Excellence

Washington University in St. Louis
Rita Parai
Seeing Through the Fission: Multi-Modal Analysis of Actinides and Noble Gas Isotopes in Geological Samples

User Facilities

Washington State University
Yogendra Gupta
Dynamic Compression of Materials: Multiscale Measurements and Analysis

High Pressure Collaborative Access Team
Nenad Velisavijevic, Director (LLNL)
Argonne National Laboratory

Fellowships

Krell Institute
Computational Science Graduate Fellowship
Laboratory Residency Graduate Fellowship
Stewardship Science Graduate Fellowship

High Energy Density Laboratory Plasmas

Cornell University
Gennady Shvets
Theory and Modeling of the Physics of Relativistic Shocks and Fermi Acceleration, and of Their Implementation Under Laboratory Conditions Using Petawatt Laser Systems

Idaho State University
Jon Stoner
Pulsed-Power Driver to Generate and Measure HED States

Johns Hopkins University
Pia Valdivia
Development of Talbot-Lau Phase-Contrast X-ray Diagnostics for High Energy Density Laboratory Plasmas

Polymath Research Inc.
Bedros Afeyan
Resonant Excitation and Multi-Stage Re-Amplification of Nonlinear Plasma Waves with Ultrafast High Energy Density Applications

Princeton University
Nathaniel Fisch
Fundamental Issues in the Interaction of Intense Lasers with Plasma

The Ohio State University
Douglass Schumacher
A Novel Study of Warm Dense Matter Using Hybrid PIC/MD Simulation Approaches Combined With Hybrid Ultrafast DAC-Based Experiments

University of California, Los Angeles
Chan Joshi
Development of a Self-Modulated Laser Wakefield Accelerator Platform for a Hyper-Spectral Photo Source from 10 KV to 1 MV for HEDS

University of California, San Diego
Christopher McGuffey
Characterization of Ion-Heated Warm Dense Matter and Its Ion Transport Properties

University of Nevada, Reno
Roberto Mancini
Atomic Kinetics of Laboratory Photoionized Plasmas Relevant to Astrophysics

University of Nevada, Reno
Alla Safronova
Hard and Soft X-ray Line Emission from High-Z Multiply Ionized Ions Influenced by Dielectronic Recombination and Polarization from HEDLP

University of Nevada, Reno
Vladimir Ivanov
Seeding and Evolution of Magnetohydrodynamic Instabilities of a Metal Surface Driven by Intense Current

University of Rochester
Jessica Shang
Probing HED Turbulence with Lasers and Coherent Light Sources

University of New Mexico, Albuquerque
Mark Gilmore
Seeding and Evolution of Magnetohydrodynamic Instabilities of a Metal Surface Driven by Intense Current

Virginia Polytechnic Institute and State University
Bhuvana Srinivasan
Seeding and Evolution of Magnetohydrodynamic Instabilities of a Metal Surface Driven by Intense Current

West Virginia University
Mark Koepke
Spectroscopic Methods for Obtaining Plasma Parameters Applied to Soft X-ray Absorption Spectra from Radiatively Heated Z-pinch Plasmas

National Laser Users' Facility

General Atomics
Christine Krauland
Characterization of the Nonlinear Laser-Plasma Interaction in Electron-Assisted Shock Ignition

Johns Hopkins University
Pia Valdivia
Demonstration of Monochromatic Talbot-Lau X-ray Deflectometry (TXD) Electron Density Diagnostic in Laser Target Interactions

Johns Hopkins University
June Wicks
High Pressure and Temperature Polymorphism of a Key Super-Earth Mantle Material: MgO

Massachusetts Institute of Technology
Richard Petrasso
High-Energy-Density Physics, Laboratory Astrophysics, and Student Training on OMEGA

University of California, San Diego
Farhat Beg
Charged Particle Transport and Energy Deposition in Warm Dense Matter with and without an External Magnetic Field

University of California, San Diego
Farhat Beg/Christopher McGuffey
Driving Compressed Magnetic Field to Exceed 10 kT in Cylindrical Implosions on OMEGA

Rice University
Edison Liang
Collision of Two Magnetized Jets Created by Hollow Ring Lasers

University of Chicago
Don Lamb
Fundamental Astrophysical Processes in Radiative Supersonic MHD Turbulence

University of Michigan
Karl Krushelnick
The Dynamics of Strong Magnetic Fields Generated by Relativistic Laser Plasma Interactions using OMEGA EP

University of Michigan
Louise Willingale
Direct Laser Acceleration of Elections for Bright, Directional Radiation Sources

University of Nevada, Reno
Roberto Mancini
A Laboratory Photoionized Plasma Experiment at OMEGA EP

Predictive Science Academic Alliance Program III

Massachusetts Institute of Technology
Youssef Marzouk
Center for the Exascale Simulation of Material Interfaces in Extreme Environments

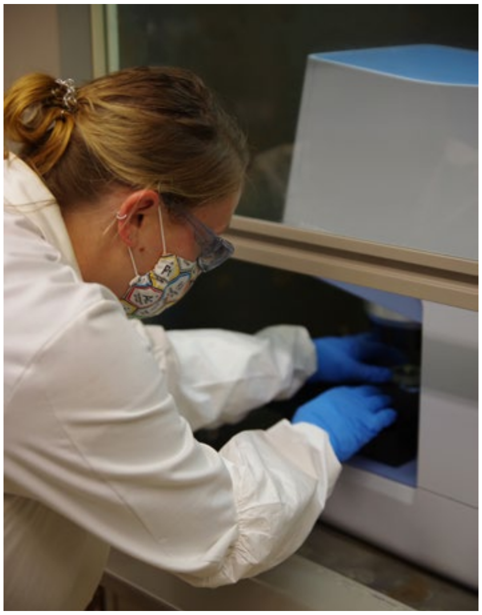
Oregon State University
Todd Palmer
Center for Exascale Monte Carlo Neutron Transport

Stanford University
Gianluca Iaccarino
Integrated Simulations Using Exascale Multiphysics Ensembles

University of Buffalo
Paul DesJardin
Center for Exascale Simulation of Hybrid Rocket Motors

University of Colorado
Richard Regueiro
Center for Micromorphic Multiphysics Porous and Particulate Materials Simulations with Exascale Computing Workflow

University of Illinois
Jonathan Freund
Center for Exascale-Enabled Scramjet Design



University of Maryland
Johan Larsson
Solution-Verification, Grid-Adaption and Uncertainty Quantification for Chaotic Turbulent Flow Problem

University of New Mexico
Patrick Bridges
Center for Understandable, Performant Exascale Communication Systems

University of Texas
Robert Moser
Exascale Predictive Simulation of Inductively Coupled Plasma Torches

Minority Serving Institutions Partnership Program

American Higher Education Consortium
Al Kuslikis
Advanced Manufacturing Network (AMFN)

University of the District of Columbia
Pawan Tyagi
Additive Manufacturing Post Processing Partnership (AMP3)

Florida International University
Shekhar Bhansali
Advanced Sensors Technologies for Applications in Electrical Engineering - Research and Innovation Excellence Consortium (ASTERIX)

Florida A&M University
Charles Weatherford
Consortium for High Energy Density Science (CfHEDS)

SUAGM, Inc. dba Universidad Ana G. Méndez-Gurabo
Amaury Malave
Consortium Hybrid Resilient Energy Systems (CHRES)

University of Texas, San Antonio
Kelly Nash
The Consortium on Nuclear Security Technologies (CONNECT)

Prairie View A&M University
Gina Chiarella
Energy Sciences: Experimental and Modeling (ESEM)

North Carolina Central University
Abdennaceur Karoui
Consortium for Nuclear Security Advanced Manufacturing Enhanced by Machine Learning (NSAM-ML)

University of Arizona
Salim Hariri
Partnership for Proactive Cybersecurity Training (PACT)

University of Texas at El Paso
Yirong Lin
Partnership for Research and Education Consortium in Ceramics and Polymers (PRE-CCAP)

North Carolina A&T University
Sameer Hamoush
Pipeline Development of Skilled Workforce in STEM through Advanced Manufacturing (STEAM)

North Carolina A&T University
Gregory Monty
Successful Training and Effective Pipelines to National Laboratories with STEM Core (STEP2NLs)

Alabama A&M University
Stephen Egarievwe
Scholarly Partnership in Nuclear Security (SPINS)

LRGF

DEPARTMENT OF ENERGY
NATIONAL NUCLEAR SECURITY ADMINISTRATION

LABORATORY RESIDENCY GRADUATE FELLOWSHIP

The Department of Energy National Nuclear Security Administration Laboratory Residency Graduate Fellowship (DOE NNSA LRGF) provides outstanding benefits and opportunities to U.S. citizens who are entering their second (or later) year of doctoral study to work at premier national laboratories while pursuing degrees in fields relevant to the stewardship of the nation's nuclear stockpile.

LAB RESIDENCY Fellowships include at least two 12-week research residencies at Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Sandia National Laboratories, or the Nevada National Security Site. Fellows are encouraged to extend these residencies to carry out thesis research and other studies at the DOE NNSA facilities.

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FIELDS OF STUDY

ENGINEERING & APPLIED SCIENCES	pulsed power; particle accelerator physics and design; detector and data processing; fluid mechanics
PHYSICS	atomic, nuclear and plasma physics; shock physics
MATERIALS	additive materials; dynamic materials; energetic materials physics and chemistry
MATHEMATICS AND COMPUTATIONAL SCIENCE	multiscale, multiphysics theory and numerical simulation; PIC/fluid hybrid simulation

BENEFITS

- $36,000 yearly stipend
- Payment of full tuition and required fees
- Yearly program review participation
- Annual professional development allowance
- Two or more 12-week-minimum national laboratory residencies
- Renewable up to four years

PHOTO: At the National Ignition Facility at Lawrence Livermore National Laboratory, a fully assembled target for laser ignition experiments incorporates a tented capsule, hohlraum, thermal-mechanical package, and silicon cooling arms.

This equal opportunity program is open to all qualified persons without regard to race, gender, religion, age, physical disability or national origin.

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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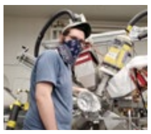
Cover Photo Captions

Cover

Senior graduate student and LRGF 2020 award winner Patty Cho at work near the center section of the Z machine.

Chad Ummel couples the GODDESS ionization chamber to the scattering chamber containing the Oak Ridge Rutgers University Barrel Array (ORRUBA) in preparation for an experiment at the National Superconducting Cyclotron Laboratory.

University of California, San Diego Graduate student Apsara Williams sets up the gas puff load on the CESZAR current generator.



Caleb Benetti (CENTAUR graduate student, FSU) stands in front of the FSU clover array, getting ready for the installation of Clarion2.

Lauren Poole investigates the dynamic behavior of biphase composites using the Split Hopkinson Pressure Bar at UCSB).

A University of Wisconsin student reconfigures and inspects the Wisconsin Vertical Shock Tube.

Back Cover

Ahmed Elshafiey of Cornell University set the controls for COBRA in the Laboratory of Plasma Studies.

Postdoctoral researchers Lee Suttle and Eleanor Tubman prepare a magnetic reconnection experiment on the Imperial College MAGPIE generator as part of the Cornell University led Multi-University Center of Excellence for Pulsed Power Driven HED Science, funded by NNSA's SSAA.

Imani Ballard preparing a Design of Experiments tribological test for a Plasma Enhanced Chemical Vapor Deposited Diamond Like Carbon Coating (PECVD DLC) technology insertion study.

CENTAUR TAMU Graduate student Austin Abbott (CENTAUR, TAMU) prepping a vacuum chamber to test DAPPER silicon detector.

Graduate student conducting research in the Institute for Shock Physics at Washington State University.

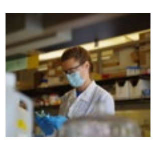
Graduate student Travis Bejines and Idaho State Accelerator Center Engineer Brian Berls assembling the 4-Brick Cinco generator.

Postdoctoral researcher conducting research in the Institute for Shock Physics at Washington State University.

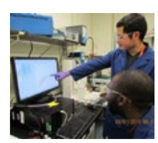
Sylvia Hanna of Northwestern University searches for single crystals of actinide metal-organic frameworks under a microscope

University of Notre Dame postdoctoral scholar Danielle Hutchison preparing to collect single-crystal X-ray diffraction data for an actinide compound at high pressure in a diamond anvil cell.

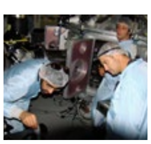
Graduate students Maxwell Sorensen and Austin Abbott (CENTAUR, TAMU) inserting a parallel-plate avalanche counter into a testing chamber.



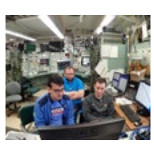
University of Notre Dame PhD student Sara Gilson calculating the number of moles for synthesis of an actinide metal organic framework (MOF).



Luis Angel Chavez Atayde, Los Alamos National Laboratory, working with fellow MSIPP student on data analysis of a novel energy conversion methods.



Graduate student Krish Bhutwala (UC San Diego), research scientist Mario Manuel (General Atomics), and post-doctoral scholar Mathieu Bailly-Grandvaux (UC San Diego) set up an optical streak camera for magnetized laser plasma interaction experiment at the Jupiter Laser Facility at LLNL.

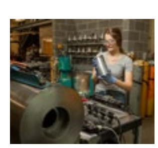


Experiment with the NEXT neutron detector at Edwards Accelerator Laboratory at Ohio University with Joe Heideman, Shree Neupane and Josh Hooker from The University of Tennessee.

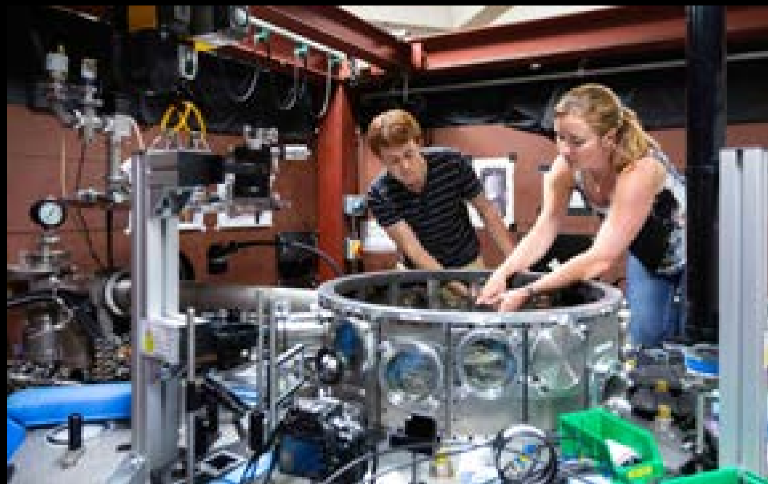
Ashabari Majumdar, a graduate student from the Nuclear Science Laboratory at the University of Notre Dame, is measuring the activity of actinide targets.

VANDLE experiment at RIBF RIKEN in Japan (The University of Tennessee Knoxville).

Rutgers University PhD student Harry Sims and the Oak Ridge Rutgers University Barrel Array



Undergraduate student conducting research in the Institute for Shock Physics at Washington State University.

RSC