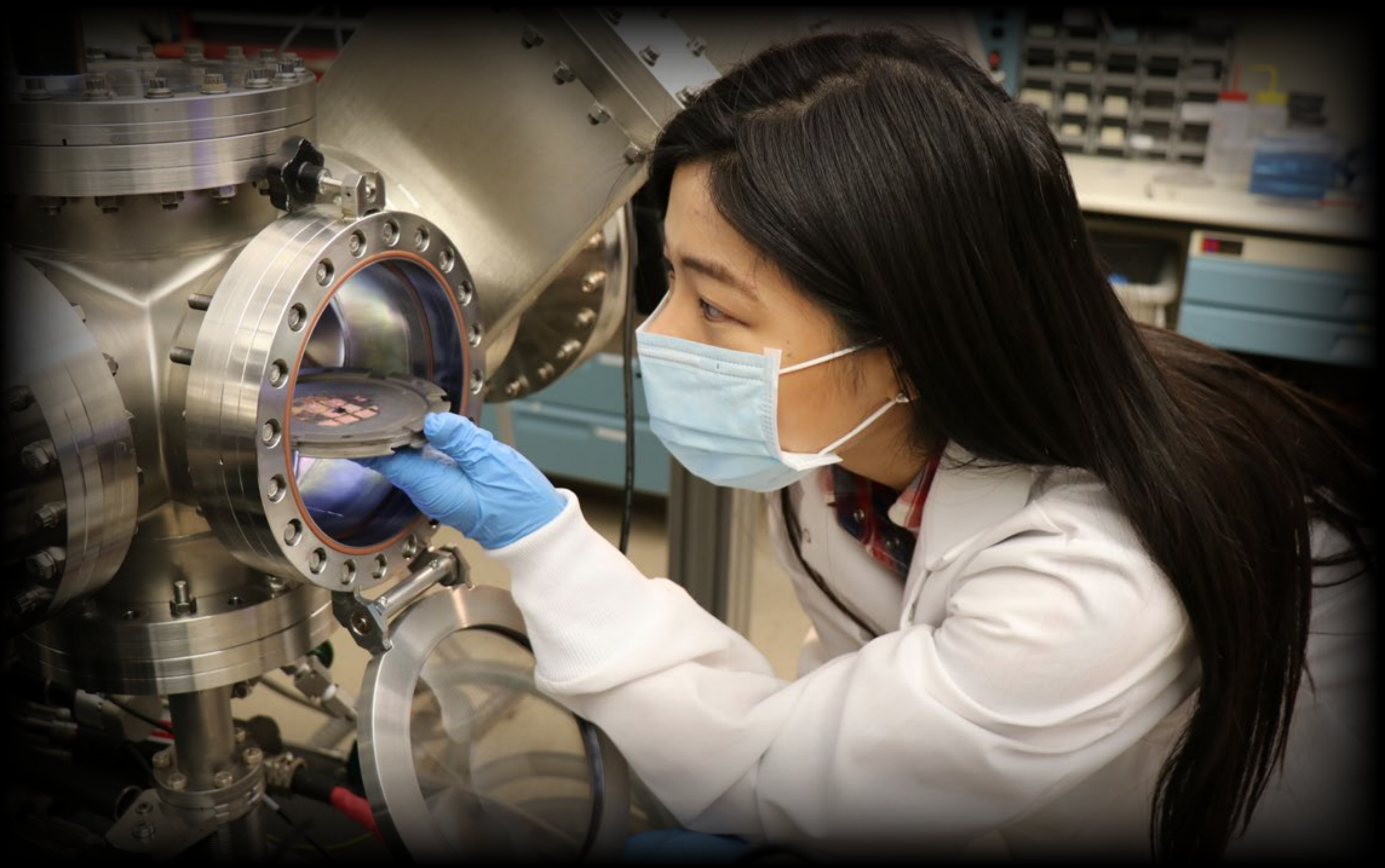
DOE/NA-0126

2022
Academic Programs Annual

Office of Research, Development, Test, and Evaluation

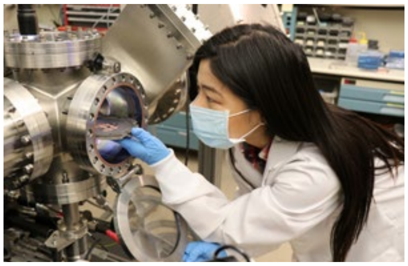
- Stewardship Science Academic Alliances
- High Energy Density Laboratory Plasmas
- National Laser Users' Facility
- Predictive Science Academic Alliance Program III
- Minority Serving Institutions Partnership Program
- Fellowship Programs



National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY

On the Cover



PhD student Emmeline Sheu, Texas A&M University Center for Research Excellence on Dynamically Deformed Solids, loads a deposition holder at the Center for Integrated Nanotechnologies at Los Alamos National Laboratory.

— Image courtesy of Texas A&M University

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NNSA Office of Research, Development, Test, and Evaluation

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The *Academic Programs Annual* is produced by the NNSA Office of Research, Development, Test, and Evaluation. It features select research conducted by the following NNSA-supported research programs: Stewardship Science Academic Alliances, High Energy Density Laboratory Plasmas, National Laser Users' Facility, Predictive Science Academic Alliance Program III, the Minority Serving Institutions Partnership Program, and fellowship programs.

Please submit comments to:

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Published February 2022

> *"Nuclear deterrence has been shown to be effective, but it must be strengthened continually through the development of world-class, state-of-the-art science and technology along with training and recruiting top talent to serve as the next-generation of nuclear stewards. This is the vital role that the SSAP serves, and we are especially grateful for our community members who have gone on to careers with the national laboratories."*

— 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

As I sit down to write, the breaking news is about an even more contagious variant of the COVID-19 omicron strain that is emerging on the heels of the first omicron variant. We continue to face this pandemic crisis and all of the anxiety and loss associated with it. My best thoughts are to focus on community and how we can bolster each member of our community to collectively achieve the greater good. The Stewardship Science Academic Programs (SSAP) community is a special and strong one. We work in partnership with U.S. academia, the National Nuclear Security Administration (NNSA), and the NNSA national laboratories to foster and grow scientific and technical excellence in the interest of national security. It is a community made up of top talent in scientific and technical disciplines that serve the vital interests of our Nation. Being a member of this community is one the most satisfying aspects of my career. Thanks to the support of our community, last year's unprecedented, virtual symposium was a great success. This year's virtual symposium will be sure to top it, even if we all would prefer to meet in person. Let's hope we will be able to next year.

This is the 30th year of conducting the nuclear weapons program without needing to perform underground nuclear testing. Everyday we have evidence that our efforts in stewarding the nuclear stockpile with science are keeping the United States, its allies, other friends, and the world-at-large safe through deterrence. Nuclear deterrence has been shown to be effective, but it must be strengthened continually through the development of world-class, state-of-the-art science and technology along with training and recruiting top talent to serve as the next-generation of nuclear stewards. This is the vital role that the SSAP serves, and we are especially grateful for our community members who have gone on to careers with the national laboratories.

The value of the work that our community does to build a safer world is evident in the pages of this Annual. We feature select students pursuing doctoral degrees and alumni of the SSAP who write in their own words about their experiences with SSAP and the opportunities that it has afforded them. We are honored to have all of you as part of our community, and I extend to each of you my congratulations for your successes to date and anticipation for your success in the future. Let's continue to work together to keep this community and, in turn, the Nation thriving and strong.

Keep yourselves and your loved ones safe,

Dr. Mark C. Anderson

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

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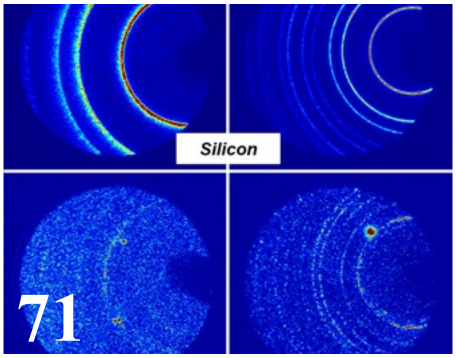

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The Academic Programs enable a robust and diverse research and science, technology, engineering, and mathematics (STEM) educational community through a variety of methods of support.

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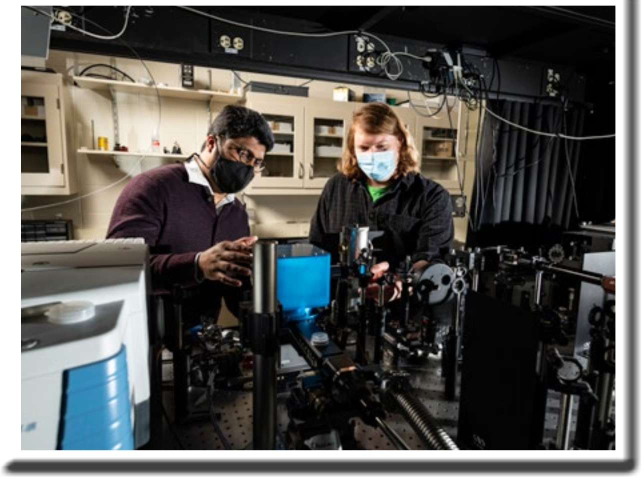
Overview



Academic Programs

Office of Research, Development, Test, and Evaluation

— 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.

Center for Research Excellence on Dynamically Deformed Solids (CREDDS, Texas A&M University) PhD student Avery Samuel (University of California, Santa Barbara) installs a high-speed camera on a split-Hopkinson pressure bar.

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:

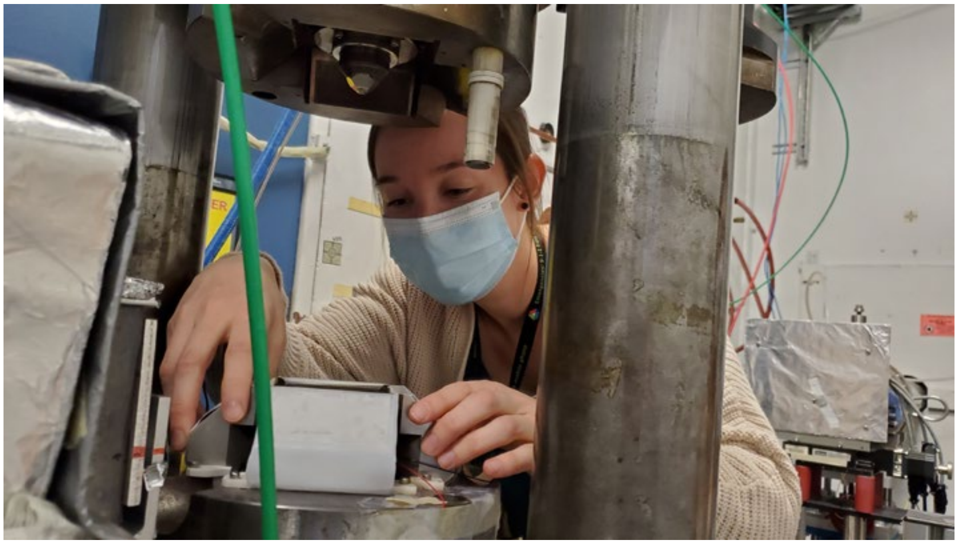
- Stewardship Science Academic Alliances
- High Energy Density Laboratory Plasmas
- Predictive Science Academic Alliance Program
- Minority Serving Institutions Partnership Program
- Fellowship Programs

Stewardship Science Academic Alliances

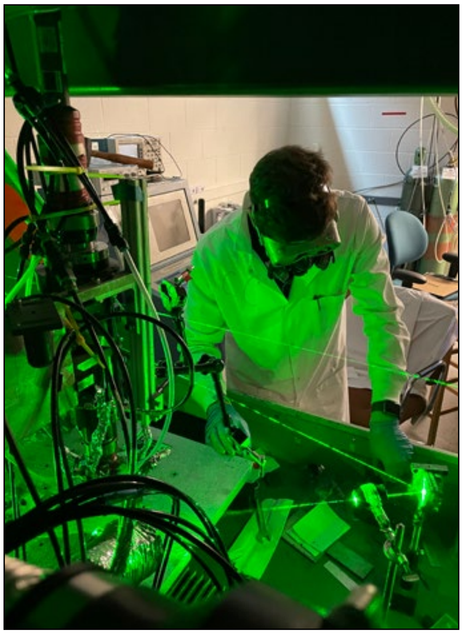
The Stewardship Science Academic Alliances (SSAA) Program supports scientific academic research programs to develop the next generation of highly trained, technical workers able to support its core mission and to ensure there is a strong community of technical peers, external to the NNSA national laboratories,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

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 more than 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.

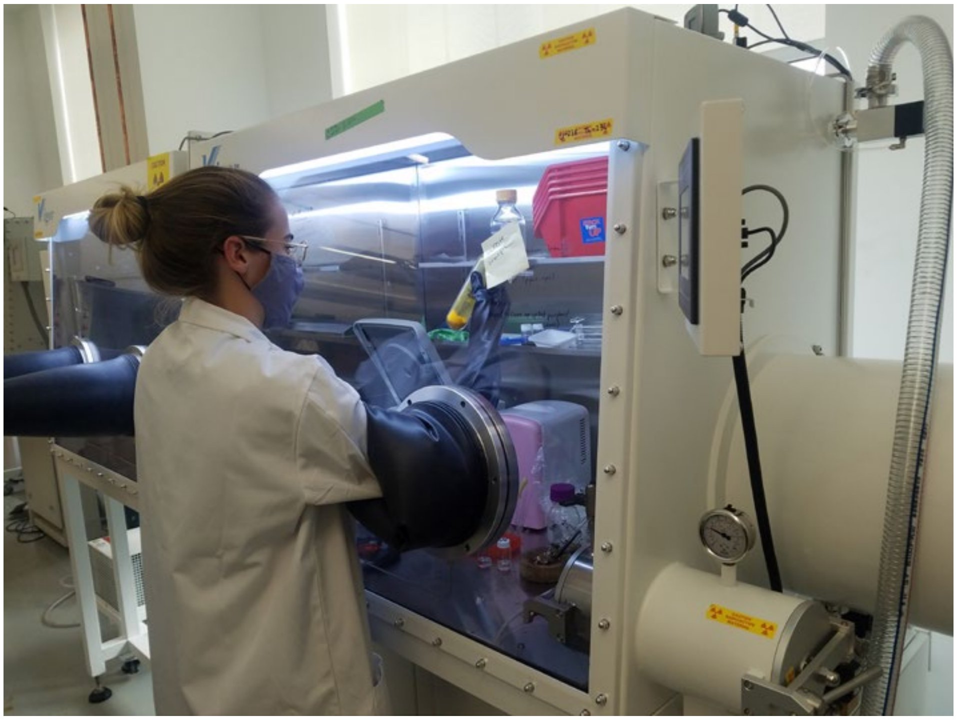
Students Julia Jitkov, Washington State University (WSU), and Ian Ocampo, Princeton University, discussing laser interferometry measurements at the Institute for Shock Physics, WSU.



University of Nevada Las Vegas PhD student Taryn Traylor positioning the DDIA anvils in preparation for an experiment measuring the change in sound velocity of SiO_2 at high pressure under compressive stress. She is working at the Advanced Photon Source sector 6 (6BM-B) using the COMPRES supported multianvil apparatus.



CREDDS PhD student Daniel Rubio-Ejchel (University of Michigan) operates a laser direct metal deposition machine for 3D printing of multiphase metallic materials.



Natalie Yaw, first year PhD student in the Actinide Center of Excellence at the University of Notre Dame, prepares a nanoparticle synthesis reaction using UO2(acac)2 (the yellow-orange compound) as a solid-state precursor, which she synthesized as a starting material. The synthesis is run under an inert atmosphere to provide precise control over the oxidation state of the as-synthesized constructs.

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.

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 JPHEDLP 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 Users' Facility

The primary purpose of the National Laser Users' Facility (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.

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.

Minority Serving Institutions Partnership Program

The Minority Serving Institutions Partnership Program (MSIPP) and Tribal Education Partnership Program (TEPP) are vital programs within the DOE/NNSA Management and Budget office, under Learning and Career Management. MSIPP/TEPP award grants to Minority Serving Institutions (MSI), who partner with national laboratories and plants, to build a diverse and sustainable technical pipeline to prepare NNSA's science, technology, engineering, and mathematics (STEM) next-generation workforce. The program aligns investments in university capacity and workforce development with DOE/NNSA mission areas to develop the needed skills and talent for DOE/NNSA's enduring technical workforce and to enhance research and education at MSIs.

2019-2020 LRGF and SSGF Classes. Left to right: Eldred Lee, LRGF; Dane Sterbentz, LRGF; Ryan Childers, LRGF; Lauren Smith, SSGF; Patrick Adrian, SSGF; David Chin, SSGF; Sylvia Hanna, SSGF; and Justin Cheng, SSGF. Not pictured: William Brooks, LRGF.

Funding for the program is identified in the National Defense Authorization Act. In FY22 MSIPP/TEPP appropriations amounted to $50 million. Since 2019, the funding for the program has increased by 125 percent, and has resulted in the program increasing partnerships by 300 percent (6 consortia in 2019 to 24 consortia with 46 schools in FY 21). MSIPP is expected to grant 6 new awards in FY22.

The program's mission is to create and foster a sustainable STEM-pipeline that prepares a diverse workforce of world class talent through strategic partnerships between MSIs and the Nuclear Security Enterprise (NSE). To execute this mission, MSIPP/TEPP build a network of NSE ready students through enrichment activities from K–20 to postdoctoral level. Through university-national lab consortia partnerships students are exposed to cutting-edge research and activities in their relevant fields.

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 four critical goals:

1. Strengthen and expand minority and tribal serving institutions' educational and/or research capacity in NNSA mission areas of interest.
2. Target collaborations and increase interactions between minority, tribal serving institutions, labs, and M&O partners to increase 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 exposure experience 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.

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, extern-ships, 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.

DOE/NNSA Fellowship Programs

The Academic Programs also include 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.

> *“This joint effort provides a unique opportunity for the Centers’ students and postdoctoral scholars to work as a team, to exchange ideas, and to take maximum advantage of the diagnostic suite on the COBRA facility.”*

— *Dr. Farhat Beg, David Hammer and Bruce Kusse*
University of California, San Diego and Cornell University

Featured Academic Collaborations

Academic Programs Supports the Stockpile and Recent Significant Inertial Confinement Fusion Advance

Dr. Annie Kritcher (kritcher2@llnl.gov) and Dr. Alex Zylstra (zylstra1@llnl.gov) ✦ Lawrence Livermore National Laboratory

The recent National Ignition Facility (NIF) HYBRID-E experiment, N210808, and follow-on experiments mark a significant advance in inertial confinement fusion research. In this experiment, for the first time, the energy released from fusion was greater than that imparted to the capsule and yielded a total fusion energy of 1.35MJ, entering a new regime of thermonuclear burn. This platform will be crucial in testing our best simulation models and understanding the physics of thermonuclear burn in lieu of testing. This result also will be used as a neutron source for stockpile stewardship applications.

The decades of effort to make this result a realization have benefited greatly from the Department of Energy/National Nuclear Security Administration's (DOE/NNSA's) Stewardship Science Academic Programs (SSAP) in multiple areas. Among these are attracting and training a pipeline of scientists to maintain the strategic deterrent.

Lead designer for these experiments, Annie Kritcher, participated in experiments and data analysis that was enabled by the High Energy Density Laboratory Plasmas and National Laser User Facility programs when she first joined the laboratory as a student. She stated, "these collaborations and experimental opportunities are what attracted me to the laboratory. The alliances with universities remain a high attraction point and is important for maintaining the scientific culture of the lab."

Experimental lead, Alex Zylstra, and shot Responsible Individual, Dan Casey, also participated in these programs completing their thesis' within R. Petrasso's group at the Massachusetts Institute of Technology, a group deeply involved through the Stewardship Science Academic Alliance (SSAA) in analyzing NIF data and developing diagnostics for understanding NIF implosions. Alex also was a DOE/NNSA Stewardship Science Graduate Fellow during his PhD and says that "[t]he opportunities to work on [high energy density] physics as a graduate student and [to] interact with the excellent scientists at the national labs is what set me on the career path to where I am today."

Figure 1. Lead Experimentalist Alex Zylstra and Lead Designer Annie Kritcher with an example ICF target.

> *"Alex also was a DOE/NNSA Stewardship Science Graduate Fellow during his PhD and says that "the opportunities to work on high energy density physics as a graduate student and to interact with the excellent scientists at the national labs is what set me on the career path to where I am today.""*

Another member of the team, C. Weber, who generates high resolution simulations of the implosion and improves modeling capabilities, was supported and brought to the laboratory under the SSAA program. Collaboration with universities increases understanding of implosions and acts as a pipeline for the next-generation of scientists, Students of S.H. Glenzer have won the Stewardship Science Graduate Fellowship and the Laboratory Residency Graduate Fellowship and will be trained in a relevant physics area. Discussions with S.H. Glenzer and team have been important for these results. Another example is the group of R. Betti's at the Laboratory for Laser Energetics who benefit from SSAP funding and have funneled important members of the NIF team to the laboratory. Following the result of N210808, the interest among young scientists has risen significantly and many of these young scientists likely will benefit from the DOE/NNSA SSAP program.

The results from this work have been accepted to *Nature* and *Nature Physics* and will be submitted to *Physical Review Letters*. Publishing these results in prestigious journals is important for attracting young talent to these areas of research and for recruiting young talent to the DOE/NNSA national laboratories.

Collaborative Experiments on Gas Puff Z-pinches between Two Centers of Excellence

Center for Matter Under Extreme Conditions, PI: Dr. Farhat Beg (fbeg@eng.ucsd.edu) ✦ Multi-University Center of Excellence for Pulsed-Power-Driven, High-Energy Density Science, Co-PIs: David Hammer (dah5@cornell.edu) and Bruce Kusse (brk2@cornell.edu)

Gas puff Z-pinches have applications in radiation physics, thermonuclear fusion, materials studies, and as fundamental research on high energy density plasmas[1]. However, mitigating the detrimental Magneto-Rayleigh-Taylor Instability (MRTI) and developing a comprehensive understanding of implosion dynamics are challenging research issues that must be tackled. The two Stewardship Science Academic Programs (SSAP) Centers of Excellence named above have undertaken a joint experiment addressing MRTI mitigation and the determination of the thermal conductivity in gas-puff Z-pinches on Cornell University's COBRA 1 MA, 200 ns generator. Originally proposed by University of California San Diego (UCSD) researchers to take advantage of the Thomson scattering and other synchronized diagnostics at Cornell, it was delayed by more than a year by COVID-19 restrictions. The recent set of experiments, jointly designed by UCSD project scientist Fabio Conti and Cornell research associate E. Sander Lavine, were successfully completed in September 2021 (Figure 1).

One primary objective of these experiments was to investigate techniques to mitigate MRTI, an instability inherent to imploding Z-pinches that develops when a lighter fluid, the vacuum magnetic field, accelerates a heavier fluid, the plasma itself. Effective strategies include tailoring the initial density profile using multiple concentric gas-shells and a central jet 'target'[2,3] and embedding an axial magnetic field (Bz) in the load[3,4,5]. Magneto-hydrodynamic (MHD) simulations predict that combining these approaches could be advantageous and could lead to higher stagnation temperatures and densities[6]. MHD numerical results indicate that the initial Bz required to adequately stabilize a double-shell implosion is about half the value needed to stabilize a single-shell due to a "reset" of the instability that occurs when the two gas shells merge[6]. To monitor the MRTI growth, multiple self-emission imaging methods were fielded. A comparison of single and double shell-on-target implosions both with and without Bz was conducted.

The single-shell configuration showed large amplitude instability without axial magnetic field, but the pinch exhibited stable behavior with an external field of Bz = 0.3 T. The double-shell configuration, on the other hand, showed stable behavior with Bz = 0.1 T, as shown in 1 This trend is consistent with two-dimensional (2D) MHD simulations.

Figure 1. Dr. Fabio Conti of UCSD (foreground) and Dr. Sander Lavine of Cornell working on load hardware for the axial magnetic field system during the joint experiment on COBRA.

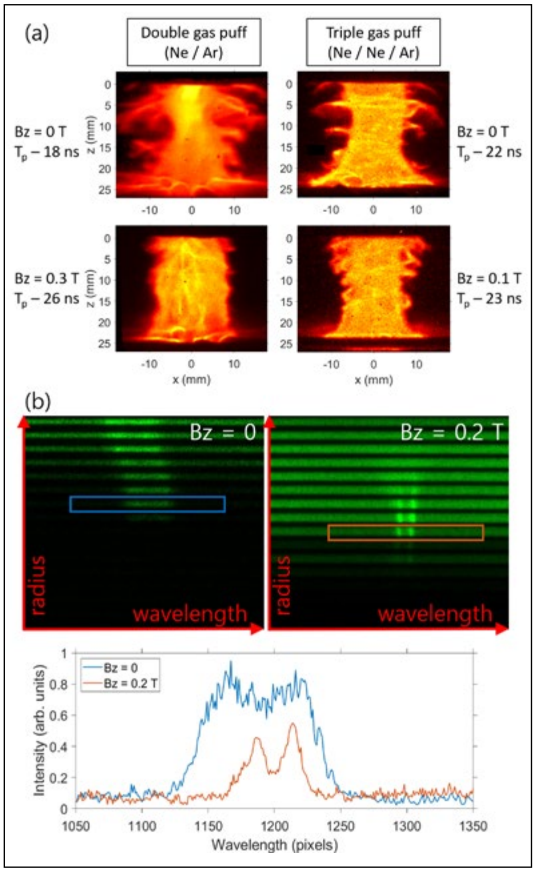


Figure 2. (a) Extreme-ultraviolet self-emission images of double (left) and triple (right) gas puff Z-pinches, demonstrating a lower threshold value of Bz for instability mitigation in a triple gas puff compared to a double gas puff. (b) Thomson scattering spectra for triple gas puff without Bz (left) and with Bz (right). The raw spectra are shown on top, with selected lineouts of the ion-acoustic feature at the bottom. The case with Bz = 0.2 T shows a smaller peak separation and broadening, indicating lower temperature of the imploding plasma.

The second objective of these experiments was to measure temperature profiles across the imploding plasma sheath via Thomson scattering to determine the thermal conductivity. Plasma parameters were determined as a function of position via Thomson scattering, interferometry, and emission spectroscopy. The scattering spectra shown in Figure 2b suggests that the imploding liner is colder when a Bz is applied, as indicated by reduced spectral peak separation (electron temperature) and reduced peak broadening (ion temperature). This is in apparent contrast with simulation results in which the electrons become magnetized and hotter when a moderate Bz ≈ 0.2 T is used due to lower thermal conductivity. Deriving an experimental estimate of the thermal conductivity from radial temperature profiles is still a work-in-progress. Further analysis by students and postdoctoral researchers from both Centers is underway.

This joint effort provides a unique opportunity for the Centers' students and postdoctoral scholars to work as a team, to exchange ideas, and to take maximum advantage of the diagnostic suite on the COBRA facility.

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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.

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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)

The Cornell Multi-University Center of Excellence for Pulsed-Power-Driven, High Energy Density Science carries out current-driven high energy density (HED) plasma research at four US universities and two abroad. Our experiments elucidate the dynamics of HED z-pinch implosions with the help of theory and extended magnetohydrodynamic (XMHD) computer simulations using the PERSEUS (Cornell) and GORGON (Imperial College) codes. Here we discuss recent experimental and theoretical results.

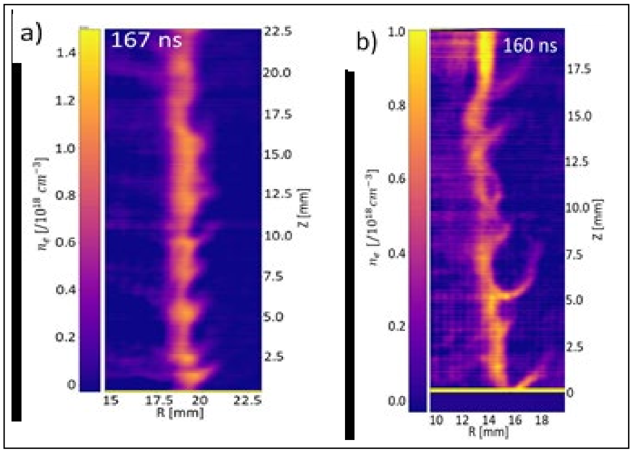

Figure 1. Experimental sheath profiles obtained from interferometry for two neon gas puff implosions a.) #5867 with plenum pressures of 2.5-6.7-17 psia in the outer-inner-center (~50 µg/cm) shows strong shock. b.) #5966 with plenum pressures of 1.4-4.2-15 psia (~25µg/cm) does not show a shock.

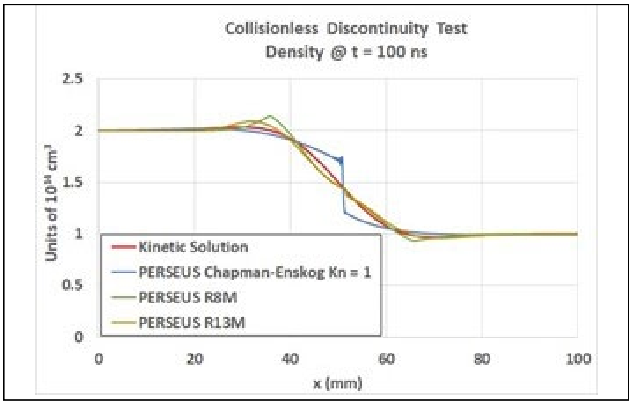

Figure 2. PERSEUS solutions compared to an analytical kinetic solution for a collisionless system. Density initialized as a 2:1 discontinuity at t = 0 & x = 50 mm. 8-moment and 13-moment models are shown as well as a 5-moment Chapman-Enskog model.

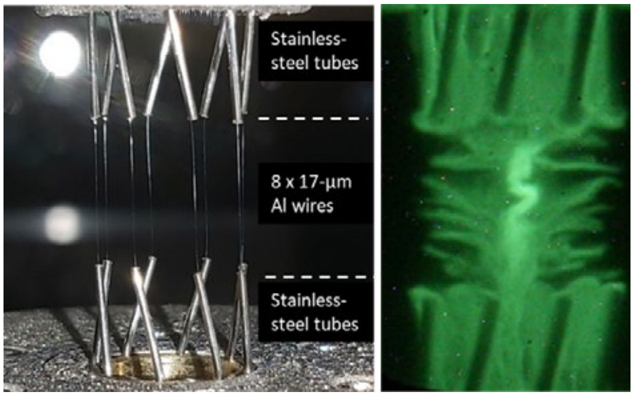

Figure 3. Dynamic magnetic mirror load for shot 6284 and an XUV self-emission image during implosion.

Experiments on the 1 MA COBRA pulsed-power machine at Cornell use Thomson scattering and laser interferometry to characterize the conditions within gas-puff z-pinches with high spatial and spectral resolution. Differences in velocity, density, and temperature profiles were observed between various gas species at similar mass density as well as identical gas species at different initial fill densities. The Thomson scattering spectra imply, in some cases, the development of hydrodynamic turbulence that may carry a significant fraction of the implosion kinetic energy. This conclusion is consistent with analysis by Center partners at Princeton and the Weizmann Institute.[1]

The profiles of the imploding z-pinch plasma sheaths fall into two distinct groups: a shock-like profile with sharp density, velocity, and temperature discontinuities at the leading edge and with minimal turbulence except at the shock front, and a shock-less profile with a gradual increase in density and velocity at the leading edge, more uniform temperatures, and significant turbulence throughout the sheath. Example density profiles determined from interferometry are shown in Figure 1. These two modes may be analogous to deflagration and detonation modes for classical combustion waves.[2] Our present hypothesis is that a transition between modes may occur at different points during the z-pinch implosion dictated by gas species and initial fill density.

Whereas most XMHD codes utilize Braginskii-like (Chapman-Enskog) transport coefficients, PERSEUS has been upgraded to solve the regularized 13-moment equations.[3] It now can handle collisionless systems where the particle distribution functions may deviate significantly from equilibrium. Anisotropic viscosity, thermoelectric effects, and thermal conductivity now can be included in simulations. In a collisionless test, PERSEUS provided a good match to the analytic solution of the Vlasov equation for one-dimensional ballistic diffusion with a 2:1 density discontinuity. Figure 2 shows the PERSEUS solutions converging to the analytic solution, as the number of moments increased from 8 to 13. By contrast, the Chapman-Enskog solution diverges in the collisionless limit (not shown in Figure 2), and even with finite collisionality (Kn=1 in Figure 2) gives an unphysical solution.

A reconfigurable wire array load that produces temporally and spatially varying axial magnetic fields has been developed. It consists of eight 17-µm diameter Al wires each threaded through semi-rigid tubes as shown in Figure 3. The top and bottom sets of tubes can be rotated with respect to each other to produce a tailored axial magnetic field. By twisting the tube sections while keeping the wires straight (Figure 1), the effect of a dynamic magnetic mirror on wire array implosion and radiation output has been studied. Such a configuration can be implemented in Magnetized Liner Inertial Fusion (MagLIF) experiments with an auto-magnetizing liner for confinement of the fusion fuel.

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Center for Advanced Nuclear Diagnostics and Platforms for Inertial Confinement Fusion and High Energy Density Physics at Omega, NIF, and Z

Massachusetts Institute of Technology ✦ PI: Dr. Chikang Li (Li@psfc.mit.edu)

A critical feature of the Center of Excellence for Advanced Nuclear Diagnostics and Platforms for Inertial Confinement Fusion (ICF) and High Energy Density Physics (HEDP) is its unique partnership of five universities with different but complementary expertise in computational, theoretical, and experimental multi-ion/kinetic physics. The strong interaction, communication, and collaboration among the Center partners and Department of Energy/National Nuclear Security Administration (DOE/NNSA) laboratories are ideal for promoting and advancing our scientific program and student training, contributing to DOE/NNSA's stockpile stewardship mission.

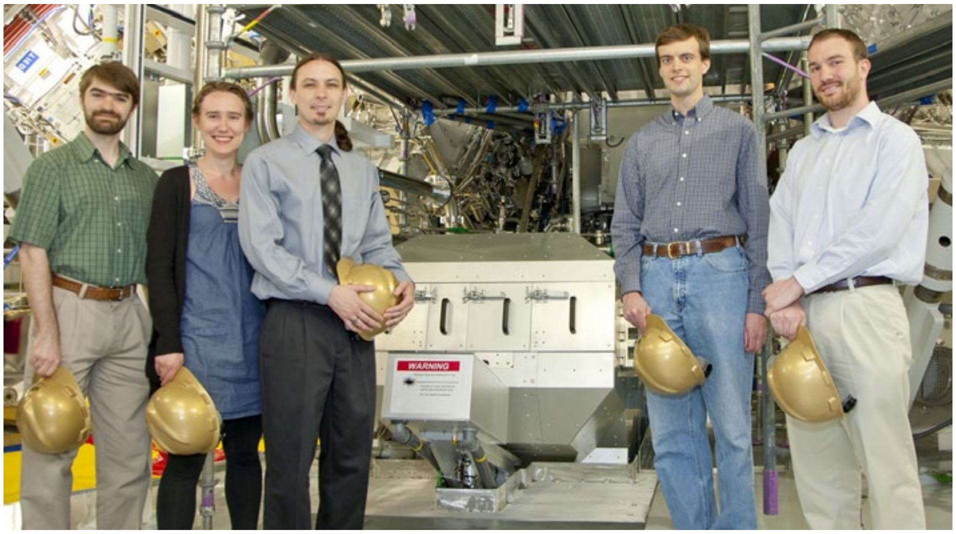

Figure 1. The MRS neutron spectrometer that was important in the record-yield NIF shot of August 8, 2021. Shown here is Dr. Maria Gatu Johnson (Research Scientist at MIT and Responsible Scientist for the NIF MRS neutron spectrometer) with former MIT students in front of the MRS. From left to right: Dr. Hans Rinderknecht (MIT PhD, 2015 and now Staff Scientist at the Laboratory for Laser Energetics (LLE)); Dr. Maria Gatu Johnson; Dr. Dan Casey (MIT PhD, 2012 and now Staff Scientist at LLNL), who got his PhD on the implementation and use of the MRS spectrometer; Dr. Alex Zylstra (MIT PhD, 2015 and now Staff Scientist at LLNL), who was the PI for this record implosion experiment; and Dr. Mike Rosenberg (MIT PhD, 2014 and now Staff Scientist at LLE).

The Center includes groups at the Massachusetts Institute of Technology (MIT), with Principle Investigator (PI) Chikang Li, four scientists, one postdoc, and 10 PhD students; University of Michigan (UM), with PI Scott Baalrud and a PhD student; University of Nevada, Reno (UNR) with PI Roberto Mancini and a PhD student; University of Rochester (UR) with PI Riccardo Betti and one scientist; and Virginia Tech (VT) with PI Bhuvana Srinivasan and one PhD student.

Two and a half years of Center work have facilitated new fundamental plasma research, important diagnostic development, and student recruitment and training that includes working with national laboratory mentors. Three students who earned their PhDs within the Center now work at Lawrence Livermore National Laboratory (LLNL) and Los Alamos National Laboratory (LANL), and two undergraduates have gone on to pursue HEDP PhDs. One postdoc and two PhD students will soon finish their work at MIT and are likely to apply for positions at the national laboratories.

There are strong collaborations among the Center students. Patrick Adrian (MIT) and Enac Gallardo Diaz (UNR) worked together to design and execute experiments that used Krypton L-shell emission as a spectroscopic tracer for electron density and temperature for studying charged-particle transport in dense plasmas (which is very important for basic science and ICF). To prepare for these experiments, which involved implosions of thin, glass capsules filled with D^{3}He and trace amounts of krypton, Patrick ran hydrodynamic simulations, and Enac post-processed them using UNR's population-kinetics code to optimize the measurement of Kr line emission with a specially-designed Multi-Monochromatic Imager diagnostic. They ran the experiments with the optimized configuration on the OMEGA laser and extracted krypton line information.

MIT student Ben Reichelt is collaborating with VT student Liam Welch to overcome computational constraints that limit most ICF simulations to average-ion, radiation-hydrodynamic models without multi-ion physics, including diffusive or viscous effects. They're looking at the importance of transient, nonideal effects like diffusive mix in moderately-coupled regimes, using the LANL code xRAGE, an average-ion radiation-hydrodynamic code, and Gkeyll, a suite of plasma physics solvers with a multi-ion code and full implementation of Maxwell's equations. Center partner UM is currently implementing diffusion coefficients and viscosity in Gkeyll, and comparison of the results of simple shock simulations to the xRAGE results should shed new light on effects that have been neglected in past ICF modeling, such as diffusive mix and shock release of cryogenic fuel into the hot spot.

Center scientists are making major advances in ICF and laboratory astrophysics and are providing crucial diagnostic support to the major ICF facilities: the National Ignition Facility (NIF) at LLNL, Omega (at UR), and Z (at Sandia National Laboratories). One very interesting area of ICF research being explored at Omega by Center scientists and students is how externally-imposed magnetic fields affect ion and electron transport and whether such fields can be used to enhance ICF implosion performance.

MIT has developed about a dozen diagnostics for assessing ICF implosion performance at the NIF, and one of the most important is the Magnetic Recoil neutron Spectrometer (MRS) for recording fusion-neutron yields and spectra (Figure 1). The extended dynamic range of the MRS played a pivotal role on August 8, 2021, when researchers at the NIF achieved a record ICF neutron yield of about 1.3 megajoules.

Center for Research Excellence on Dynamically Deformed Solids

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

The stockpile stewardship mission poses a major challenge to materials science and engineering: how do we synthesize advanced, multiphase materials with superior performance under rapid deformation at strain rates of 10^4/s and higher? The Center for Research Excellence on Dynamically Deformed Solids (CREDDS) addresses this question through a collaboration between four academic institutions—Texas A&M University (TAMU), University of Michigan (UM), University of California at Santa Barbara, and University of Connecticut—and the Department of Energy/National Nuclear Security Administration (DOE/NNSA) national laboratories.

CREDDS forms a tight-knit community of faculty, students, and postdoctoral researchers. Sadly, in 2021 the Center lost one of its founding members. Dr. Jyoti Mazumder, National Academy of Engineering member and professor of mechanical engineering at the University of Michigan, passed away in his hometown of Ann Arbor. Dr. Mazumder (Figure 1) commercialized direct metal deposition, an advanced materials processing method fueling the ongoing additive manufacturing revolution. “He was a pioneer in his field and an outstanding collaborator,” said CREDDS director, Michael Demkowicz. “He will be missed.”

CREDDS welcomes two new faculty members, Dr. Jerard Gordon at the University of Michigan and Dr. Ankit Srivastava at TAMU. Dr. Gordon is an expert in metal additive manufacturing. His group will ensure that CREDDS continues to lead in advanced manufacturing, including direct metal deposition methods. Dr. Srivastava focuses on microstructure-sensitive modeling of mechanical deformation. Working together, Gordon and Srivastava have initiated a new line of research on the effect of controlled porosity on high strain rate mechanical deformation. University of Michigan PhD student, Daniel Rubio-Ejchel (Figure 2), works with Dr. Gordon on synthesizing the materials needed for this investigation.

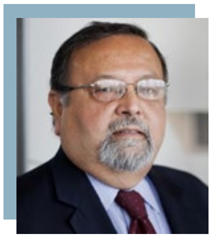

Figure 1. Dr. Jyoti Mazumder, National Academy of Engineering member and professor of mechanical engineering at the UMichigan, commercialized direct metal deposition, and advanced materials processing method that has fueled the additive manufacturing revolution.

Figure 2. UM PhD student Daniel Rubio-Ejchel, working on synthesizing the materials needed for a new line of research on the effect of controlled porosity on high strain rate, mechanical deformation.

The past year posed challenges for students doing on-site work at DOE/NNSA laboratories. Nevertheless, three CREDDS PhD students carried out extended internships with DOE/NNSA collaborators during this time. Ethan Sprague (UM) and Marco Echeverria (University of Connecticut) worked remotely with staff at Lawrence Livermore National Laboratory (LLNL). Meanwhile, Emmeline Sheu (TAMU) became the first out-of-state user to resume in-person work at Los Alamos National Laboratory’s (LANL’s) Center for Integrated Nanotechnologies (CINT) user facility. Over the past year, Sheu (Figure 3) developed innovative techniques that combine vapor deposition and physical masking to fabricate samples with finely controlled microstructure morphologies. These samples allow her to investigate the response of multiphase materials to high temperature annealing.

Figure 4. TAMU PhD student, Christopher Walker, with the new CREDDS nanoindentation instrument.

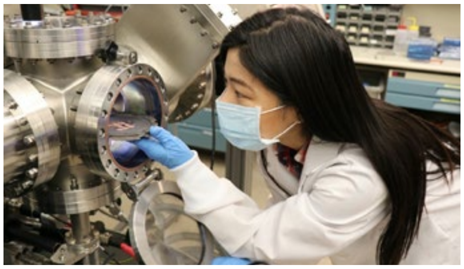

Figure 3. TAMU PhD student, Emmeline Sheu, working with LANL has developed innovative techniques that combine vapor deposition and physical masking to fabricate finely controlled microstructure morphologies.

The past year also saw notable advances in instrumentation development within CREDDS. A miniaturized, high-temperature dye for equal channel angular extrusion (ECAE) went into service at TAMU. This new tool has enabled CREDDS to explore a hitherto inaccessible range of metal microstructures. The University of California, Santa Barbara, saw the installation of an advanced, high-speed camera system that will allow researchers there to conduct quantitative analyses of high strain rate material deformation in real time. Finally, TAMU saw the completion of a novel, high strain rate, nanoindentation system. This unique tool allows CREDDS to perform high throughput measurements of mechanical response at strain rates up to 10^5/s. Figure 4 shows PhD student, Christopher Walker (TAMU), with the new nanoindentation instrument.

Thanks to outreach efforts initiated during the COVID-19 pandemic, CREDDS hosted a record-breaking number of undergraduate researchers over the past year. Twenty-six students from around the country took part in three different research programs at TAMU and the University of Michigan. In addition to engaging in technical work under the guidance of CREDDS members, these students were given opportunities to learn about stockpile stewardship through presentations and mixers with members of CREDDS and other DOE/NNSA-sponsored research projects.

The Center for Excellence in Nuclear Training And University-based Research

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

The Center for Excellence in Nuclear Training And University-based Research (CENTAUR) continues to pursue scientific excellence, while developing the future of our Nation's stockpile science workforce. Workforce development highlights include: a hybrid Scientific Advisory Committee meeting at Texas A&M University (TAMU), virtual and in-person options for the nuclear summer camp for middle school students, and a trip to Los Alamos National Laboratory (LANL) for CENTAUR students. "I'm pleased that so many of our students are going on to start rewarding careers at the [Department of Energy/National Nuclear Security Administration (DOE/NNSA)] labs," said Sherry Yennello, CENTAUR Director.

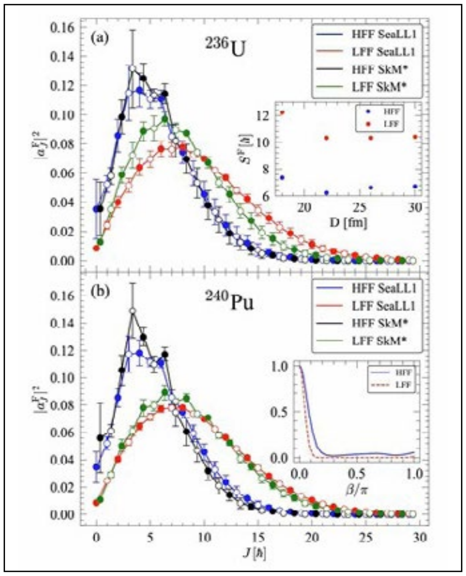

Figure 1. Calculated intrinsic spins of heavy (HFF) and light (LFF) fission fragments from induced fission of (a) ^{236}U and (b) ^{240}Pu.

Nuclear reactions involving unstable nuclei are crucial for heavy-element nucleosynthesis and the U.S. stockpile stewardship program. Recent theoretical and experimental advances have been made within the CENTAUR center. In recent work, Professor Jeremy Holt and former CENTAUR student, Dr. Taylor Whitehead, have developed, for the first-time, nuclear reaction theory models applicable across the chart of nuclides with quantified uncertainties.[1] This will enable more robust theoretical predictions for exotic nuclear reactions and estimates of associated uncertainties.

Figure 2. CENTAUR students and staff met with LANL staff at the lab in New Mexico in October 2021.

The ^{12}C(n,n')^{12}C(Hoyle) cross section, which is important in nucleosynthesis in stars, has been measured. The neutron up-scattering cross sections, which lead to enhanced production of ^{12}C in some stellar environments, were established. The main result is that the enhancement of ^{12}C production due to the neutron up-scattering is significantly smaller than the original theoretical estimate, leading to a reduced influence of this process in stellar environments. The paper has been submitted to *Nature*.

Fission is another area of interest for the center, in both experiment and theory. For more than six decades, the question of how fission fragments acquire their spins and their relative orbital momenta eluded a parameter-free microscopic treatment. This meant modeling was limited to various simple models, based on a number of unchecked assumptions and with many fitting parameters. Figure 1 shows calculations from a recent publication[2] in which a group of CENTAUR theorists from University of Washington and TAMU working with scientists from LANL and Lawrence Livermore National Laboratory (LLNL) presented, for the first time, a microscopic description of the generation of fission fragment spins and their correlations without any assumptions or fitting parameters. These predictions have been extended both within a fully-microscopic approach and a Hauser-Feshbach framework to describe further crucial details of this process. In a second work[3] performed in collaboration with scientists from LANL and University of Michigan, which was just accepted for publication in *Physical Review Letters*, the removal of angular momentum by neutrons and gamma rays from primary fission fragments was shown be crucial in understanding the results of a recent experiment.

The Nuclear Medicine and Science Camp, spearheaded by Professor Paul Cottle (Florida State University (FSU), took advantage of lessons learned from the fully-online format last year. Two camps were run in Florida: one in person and one virtually, with hands-on activities. Three camps also were run in Texas, all in person, with trips to the TAMU Cyclotron Institute and a Zoom conversation with a scientist from LANL. Overall, about 75 students participated and were exposed to different topics and career pathways in nuclear science through Center efforts.

After two planned DOE/NNSA laboratory trips that were canceled due to COVID-19 restrictions, 13 students (11 graduate and two undergraduate) involved in CENTAUR or CENTAUR-adjacent projects made the trip out to LANL at the beginning of October. They participated in a CENTAUR-LANL symposium, that consisted of talks from LANL employees and CENTAUR students, and a poster session. They heard from a panel of current LANL postdoctoral researchers, including two former CENTAUR students, and toured some LANL facilities.

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Center for Matter Under Extreme Conditions

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

The focus of the Center for Matter Under Extreme Conditions is in three thrust areas: 1) energy transport in high energy density (HED) systems, 2) material properties across HED systems, and 3) nature under extreme conditions. In the fourth year of the Center, fourteen students from University of California (UC) San Diego (UCSD), UC Berkeley, UC Davis, UC Los Angeles, University of Rochester, and Florida A&M University have worked in collaboration with the Department of Energy/National Nuclear Security Administration (DOE/ NNSA) national laboratories. Six program alumni now work at the DOE/NNSA national laboratories or at General Atomics (GA). Two projects from thrust area one are highlighted below.

One aspect of the energy transport in HED systems is aimed at understanding how lasers interact with HED plasmas in the presence of multi-Tesla magnetic fields. In a collaboration between UC Los Angeles (UCLA), UCSD, and GA, UCLA graduate student, Roman Lee, has been using the Particle in Cell (PIC) code OSIRIS to understand how stimulated, Raman scattering (SRS) is altered in the presence of 1-50 Tesla magnetic fields. In SRS, an incoming laser decays into another backward-going light wave and a forward-going electron plasma wave. Magnetic fields on the order of 10 Tesla significantly can change the dynamics of SRS, despite the fact that even for such large fields the ratio of the magnetic pressure (0.1 GPa) to the plasma pressure (500 GPa) is low. The SRS dynamics are altered due to how resonant electrons surf the electron plasma wave as a result of the magnetic field. The magnetic field causes electrons to move across the plasma wave while preventing them from outrunning the wave, leading to nonlinear damping and a more complicated nonlinear frequency shift. This can lead to a reduction in the SRS reflectivity (Figure 1). Extensive one- and two-dimensional simulations have been conducted, with current efforts being made to develop and use a quasi-three-dimensional (3D) approach for the simulations in which the problem is expanded into azimuthal harmonics of which a finite number are kept (e.g., Figure 2).

At UCSD, research involving gas-puff Z-pinches has focused on the implosion dynamics, stability, and heat transfer of double and triple concentric gas puffs. The gas-puff Z-pinch is an intense neutron and X-ray source with applications ranging from thermonuclear fusion to radiation physics and materials science.[1] However, plasma instabilities and thermal conduction losses are two important obstacles to advancing these sources. Both effects may be mitigated with a careful choice of gas puff initial parameters, namely the initial density profile, the gas species used, and the applied axial magnetic field.

Magneto-hydrodynamic (MHD) simulations show that an initial axial field of 0.7 T is expected to adequately stabilize a double gas puff implosion on a 0.9 MA, 180 ns current generator, but this condition is reduced to 0.3 T for a triple gas puff due to a “reset” of the instability that occurs when the outer gas puff merges with the middle one.[2] This reduction in required axial field by switching to a double-shell profile leads to greater compression of the center jet. Simulations also suggest that both ions and electrons can become magnetized during the implosion when an axial field is used, reducing thermal conduction losses. However, MHD models tend to underestimate the effect of the axial field.[3,4] In some experiments, instabilities can be mitigated with a field 2-4 times smaller than predicted by MHD, which warrants a systematic comparison between simulations and experiments. Additionally, using a gas species with a higher atomic number is expected to increase compressibility on one hand, while also increasing radiative losses on the other hand. The choice of gas species in the outer gas puffs, therefore, can affect the compression of the central jet, resulting in different performance for radiation production.

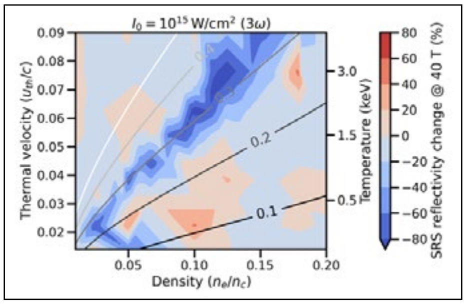

Figure 1. Parameter scan (in one dimension) showing SRS reflectivity is modified significantly by a 40T magnetic field.

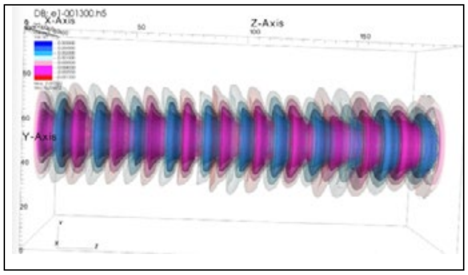

Figure 2. Geometrical effects of SRS are significant. However simulations in full three spatial dimensions can be prohibitive. Here azimuthal modes from a quasi-3D simulation are recombined to create a 3D image showing the alteration of the wavefront of SRS-driven plasma waves.

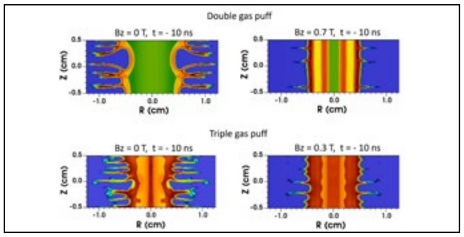

Figure 3. Stability of gas puff Z-pinch with a double or triple gas puff and applied axial magnetic field from MHD simulations with the HYDRA code. A 0.7 T and 0.3 T field are expected to reduce instability in a double and triple gas puff, respectively.

Experiments are being carried out on ~1 MA machines to test these modeling predictions by quantifying instability mitigation and thermal conduction losses as a function of applied axial field and gas species. Finding the optimal configuration at this current level can inform modeling efforts to scale this concept to higher currents.

This year UCSD hosted the 2021 HED Science Summer School (August 2-6). This online event promoted scholastic development through technical lectures given by field experts. It was attended by 90 attendees, including students and postdoctoral scholars from 41 institutions and 20 countries. Additional support and course instruction came from 29 scientists and professors. Held biannually, this marked the seventh time it had been hosted at UCSD and the first time via Zoom due to COVID-19.

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Chicago/DOE Alliance Center—A Center of Excellence for High Pressure Science and Technology

University of Illinois Chicago ✦ PI: Dr. Russell J. Hemley (rhemley@uic.edu)

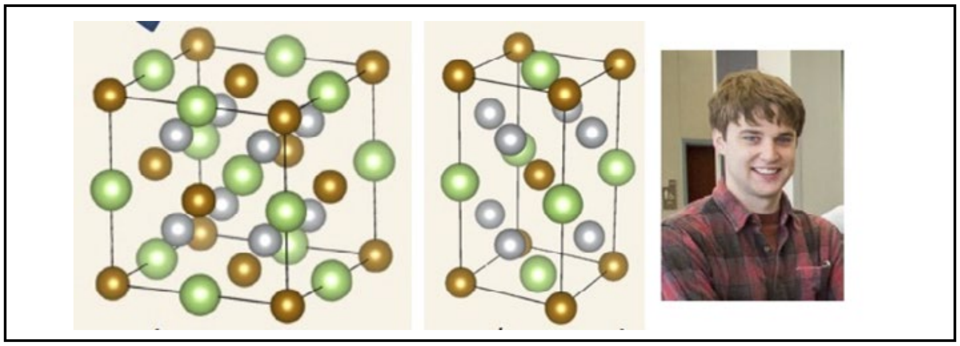

Figure 2. Left: cubic, ferromagnetic austenite $L2_1$ phase; Middle: orthorhombic, spin disordered martensite $L1_0$ phase; Right: Brian Blaneknau (University of Illinois Urbana-Champaign).

Since its founding in 2003, the mission of CDAC, now the Chicago/DOE Alliance Center, has been to enhance the understanding of a broad range of materials in extreme pressure-temperature regimes through scientific research and technique development, to integrate and coordinate static compression, dynamic compression, and theoretical studies of materials, and to facilitate the education and training of the next generation of students and postdoctoral researchers for work in science-based stockpile stewardship.

Now in its second year at the University of Illinois Chicago (UIC), CDAC continues its work in addressing a variety of key problems in extreme conditions materials science through seven science thrusts: Elasticity and Equations of State; Plasticity, Strength and Deformation; Complex Materials; Extreme Chemistry; Defects and Ion Irradiation; Phase Transition Dynamics; and Superconductivity and Electronic and Magnetic Phenomena.

CDAC Director Russell Hemley is assisted at UIC by Research Professors Stephen Gramsch (Deputy Director), Muhtar Ahart and Ravhi Kumar, who coordinate student training, outreach to a network of collaborators with shared scientific interests, and management of the laboratory facilities at UIC, which serve as a resource for the entire Center. The CDAC group also includes UIC Research Professor Zhenxian Liu, the onsite beamline scientist for the Frontier Infrared Spectroscopy Facility at the National Synchrotron Light Source II, Brookhaven National Laboratory.

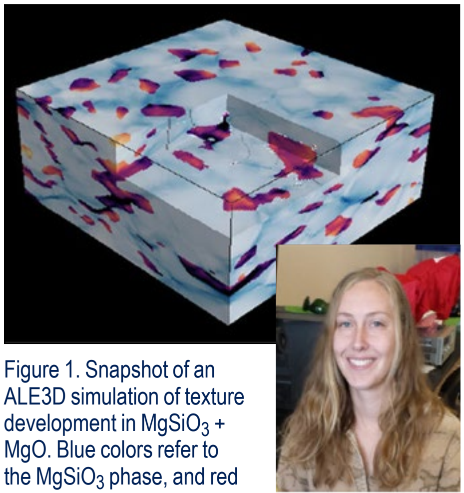

Figure 1. Snapshot of an ALE3D simulation of texture development in $MgSiO_3$ + MgO. Blue colors refer to the $MgSiO_3$ phase, and red colors refer to MgO phase. Lighter colors indicate texture development at shorter length scales, and darker colors indicate texture development at longer length scales. Lower right: Samantha Couper (University of Utah, now at LANL).

CDAC Academic Partners provide the Center with unique expertise across a wide range of topics in extreme conditions research. This group consists of Susannah Dorfman (Michigan State), Elif Ertekin (Illinois Urbana-Champaign), Steven Jacobsen (Northwestern), Maik Lang (Tennessee), Lowell Miyagi (Utah), and Eva Zurek (Buffalo). For most of its duration, CDAC has supported mainly an experimental effort, but, in recent years, the scientific program has benefitted significantly from the synergy between experiment and theory that has been made possible by the participation of CDAC Academic Partner groups utilizing first principles calculations, simulation, and modeling.

In the Miyagi group, CDAC graduate student Samantha Couper carried out experiments on texture development in a variety of single-phase materials at high pressures using radial diffraction techniques as the main focus of her dissertation research. In order to work with data on texture development in two-phase assemblages, however, it was necessary to first model the mixtures with Arbitrary Lagrangian Eulerian 3-Dimensional (ALE3D) simulations to understand the effects of microstructure on stress-strain partitioning and texture development between the two phases (Figure 1). In her collaboration with a group at LLNL, Samantha was able to develop a framework for the analysis of behavior in complex, multi-phase systems. She is now an Agnew Postdoctoral Fellow at LANL.

At the University of Illinois Urbana-Champaign, Brian Blankenau, a graduate student in the group of CDAC partner Elif Ertekin has been focusing on a theoretical description of the austenite-martensite phase transition in shape memory alloys with the Heusler composition $Ni_2Mn_{1.4}In_{0.6}$ (ideally Ni_2MnIn) with the goal of understanding the magnetostructural coupling in this class of materials (Figure 2). A key issue is how this coupling affects the dynamics and pathway of the austenite-martensite transition. A related issue under investigation is the sensitivity of the phase transition to increasing pressure. Faced with a gap in the ability of their first-principles calculations to resolve atomic positions at high pressures at a detail sufficient to reliably extract information on the phase transformation mechanism, the group has decided to carry out high pressure diffraction measurements on single crystal samples at the High Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source (APS). Brian's goal in these experiments is to obtain accurate crystal structure data with increasing pressure to inform the next phase of the calculations, specifically to address questions such as the role of phonon softening or adaptive nanotwinning in the phase transformation mechanism.

The above examples are representative of the variety of CDAC student-led projects in the Center, many utilizing synchrotron radiation, including the unique capabilities of HPCAT at APS.

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 focus of CLA is experimental, with experiments performed at a variety of HED facilities, CLA 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 the fundamental physics relevant to astrophysics in the HED regime and the [Department of Energy/National Nuclear Security Administration (DOE/] NNSA mission. We pride ourselves in the mentorship and holistic education of junior scientists in HED science.” The Center currently has eight graduate students and two postdoctoral fellows mentored by Professor Kuranz and Emeritus Professor R. Paul Drake. CLA students often work closely with scientists and engineers at the DOE/NNSA laboratories and DOE/NNSA facilities as part of their doctoral work.

Specifically, for their radiation hydrodynamics work, CLA researchers study how radiation interacts with matter. 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. Here photoionization rates must dominate over recombination rates, and recombination must dominate electron collisional ionization. Radiation-driven heat fronts are present in the early universe during reionization, the circumstellar medium of supernovae, and in HED physics experiments. Dedicated experiments to observe and diagnose the behavior of these types of heat fronts can improve our understanding of these phenomena. Currently, CLA has experimental projects exploring PI fronts on the Omega Laser Facility at the University of Rochester and the Z machine at Sandia National Laboratories. A recent simulation study of photoionization fronts using the HELIOS-CR radiation hydrodynamics code provides an experimental design for the Z machine using a measurement-calibrated input radiation flux to drive the photoionization front in a nitrogen gas.[1]

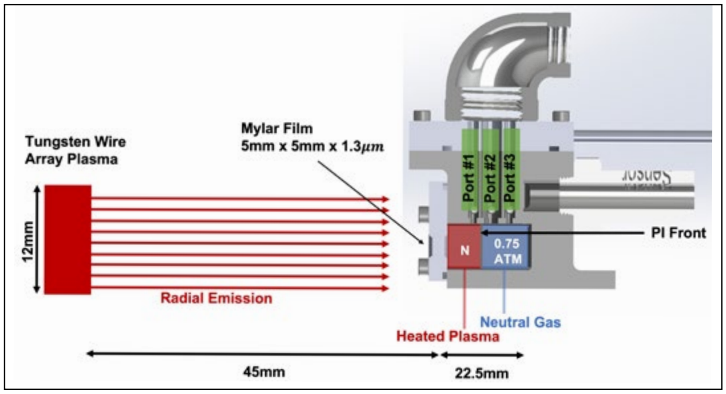

Figure 1. Schematic of the proposed experiment on the Z machine indicating key distances and diagnostics. The main diagnostics are the streaked visible spectrometer (SVS) and photonic Doppler velocimetry (PDV).

For experiments on the Z machine, the Z-pinch dynamic hohlraum (ZPDH) platform implodes a wire array creating a bright, soft X-ray source when the plasma stagnates on axis and shocks the tungsten to about 200 eV.[2] The emission from the Z-pinch plasma is incident on a N gas cell, the photons ionize the gas, and, under the correct conditions, a PI front forms and propagates in the gas. Figure 1 shows the schematic of the experiment. CLA researchers plan to use streaked, optical spectroscopy to measure the time-resolved ionization states and temperature in the heated gas. Additionally, photon Doppler velocimetry will measure the change in the index of refraction as the front propagates through the cell. From this measurement, they will be able to infer the electron density. Together, these measurements will be used to observe the changing temperature, electron density, and ionization as the heat front propagates in the gas.

Simulations to model this system used Helios-CR[3], which is a one-dimensional, Lagrangian grid, radiation, magnetohydrodynamics code with the capability of non-diffusive radiation transport and detailed atomic physics calculations. Figure 2 shows a calculated streaked spectrum using the full three-dimensional geometry conducted using SPECT3D[4] over the most relevant experimental times using the output of the Helios-CR simulations. This indicates that there is line structure early-in-time that transitions to thermal emission as the radiation continues to heat the gas as the front propagates past the fiber. The thermal emission at this point can act as a spectrally-resolved, streaked optical pyrometery (SOP) measurement. The SOP will measure the temperature as a function of time at the location of the fiber coupled to the optical spectrometer.

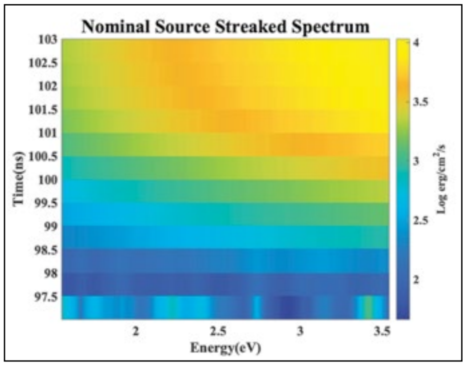

Figure 2. A calculated streaked spectrum using the Helios-CR simulations in SPECT3D. It shows line emission earlier in time which then changes to thermal emission at higher temperatures later in time (from reference 1).

CLA researchers are able to access time on the Z-machine though the Z Facility Fundamental Science Program.

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Actinide Center of Excellence

University of Notre Dame ✦ PI: Dr. Amy E. Hixon; Author: Sylvia L Hanna (sylviahanna2022@u.northwestern.edu)

Located at the foot of the periodic table lie the actinides—a family of 14 elements with seemingly ominous radioactivity, yet arguably with some of the most chemically-remarkable structures and properties. The unstable nuclei of these elements result not only in their radioactive properties but also in valuable applications including energy generation in nuclear reactors. Importantly, the actinides claim a prominent position at the Department of Energy/National Nuclear Security Administration (DOE/NNSA), as their chemistry is highly relevant to stockpile stewardship applications. For example, the study of actinides allows for an accurate, fundamental understanding of nuclear weapons components as well as the ability to predict the aging of actinide-based weapon components.

Figure 1. Fifth year PhD candidate, Sylvia L. Hanna, in the Farha group at Northwestern University handles air-sensitive, uranium-based MOF experiments in a glovebox under inert atmosphere.

Because of the clear relevance of research devoted to the actinide elements, the Actinide Center of Excellence (ACE) was founded to investigate research questions and priorities in actinide chemistry and materials that are important for the security of the Nation via stockpile stewardship, with workforce development as a motivating goal. Built from seven principal investigators and 13 students across five total institutions, ACE integrates both experimental and computational approaches to problem solving. ACE researchers investigate actinide materials ranging from the relatively docile depleted uranium and thorium isotopes to their more aggressive plutonium and neptunium counterparts via solution state, solid state, and computational methods.

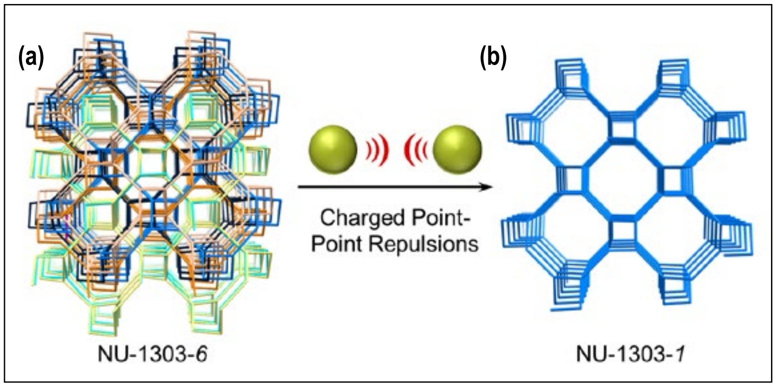

Figure 2. Fully intertwined NU-1303-6 (a) transformed to a single network of NU-1303-1 (b) via spontaneous charged point-point repulsions.

Due to structure-property relationships of this sphere of physical science at-large, new classes of materials are anticipated to produce novel properties. Likewise, new materials developed from the relatively underexplored actinide elements promise unconventional properties and unprecedented outcomes. ACE's investigation of new actinide-based materials has not disappointed in this regard. Indeed, by probing new actinide materials, a team led by the Farha group at Northwestern University in close collaboration with the Gagliardi group at the University of Chicago and others discovered a phenomenon which reverses the universal thermodynamics of stability and spontaneously creates void space from an initially crowded network system[1].

This phenomenon, termed charged point-point repulsions (CPPR) was observed in a uranium-based, porous network material called a metal–organic framework (MOF) (Figure 1). The specific MOF under analysis (NU-1303-6) is made up of six, identical, intertwined networks, such that the only way to separate the networks is to break one or more of them (Figure 2a). Such entangled structures typically are thermodynamically-favored and are pervasive in both nature and synthetic systems. However, the structure of NU-1303-6 comprises negatively charged uranium points on nearby intertwined networks, which are more closely spaced than any synthetic material observed to date. Consequently, repulsion between anionic, closely positioned uranium points (CPPR) drives the networks apart, dissolving five of the six networks spontaneously. As a result, CPPR doubles the pore size of NU-1303-6 by transforming it into its larger pore counterpart, NU-1303-1, which possesses only one network with a record high 96.6% void fraction (Figure 2b). In this manner, a new actinide-based material structure resulted in a unique occurrence and useful property of producing non-entangled structures with an abundance of valuable pore space.

Drawing on fundamental actinide chemistry, this study and similar studies within ACE enhance the DOE/NNSA mission by contributing valuable insights for stockpile stewardship. This study exemplifies the breadth of scientific space within actinide chemistry that is available for ACE students to explore. The relatively untouched field of actinide chemistry paired with the mentorship and collaborations of ACE lend the prime environment for growth and discovery. As ACE senior investigator, Omar K. Farha, remarked, “We are grateful to NNSA and ACE for the funding to keep fundamental actinide chemistry alive and offer young and talented scientists such as Sylvia the chance to discover new chemistry that only actinides can do.”

Reference

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Wootton Center for Astrophysical Plasma Properties

University of Texas at Austin ✦ PI: Dr. Donald Winget (dew@astro.as.utexas.edu)

The purpose of the Wootton Center for Astrophysical Plasma Properties (WCAPP) is solving real astrophysical problems under real astrophysical conditions. Through their experiments, astrophysics becomes an experimental science. Within recent years, the great machines like Z at Sandia National Laboratories (SNL), the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory and Omega EP at the Laboratory for Laser Energetics have made possible the creation of cosmic conditions for the first time in the sweep of human history.

The most significant growth for the Center has been the result of two interrelated things. First, the attraction of the astrophysical connections has helped spread the word at meetings and throughout the community. The Center now has grown to five graduate students and three postdoctoral researchers (postdocs). This growth has created more mentoring opportunities, including peer mentoring, and has made possible more undergraduate participation in the science of the center. In Figure 1, we show the current postdocs and graduate students. Working at the Department of Energy/National Nuclear Security Administration national laboratories has helped introduce them to the scientific culture of the national laboratories and has allowed them to perform experiments well above the academic, university, or department scale.

The increase in students and postdocs has allowed them to begin to lead the experiments and expand beyond those taking place at the Center's inception. This has motivated the use of newly-developed diagnostics and has created new growth in scientific approaches and experimental platform development. On Z, the collaboration with the Center led by Carolyn Kuranz at the University of Michigan (the Center for Laboratory Astrophysics) also has created new growth. There now are five instead of four astrophysically-motivated experiments fielded on each Z shot. This leverages the scientific impact of Z even further.

Some significant recent progress on Z has measured accretion disk conditions and has shown that the complex astrophysical models do not correctly predict the measured conditions in the laboratory. Other, complementary experiments show that Radiative Re-Combination experiments in a photoionized plasma give a powerful new way to measure temperatures in astrophysical accretion disks.

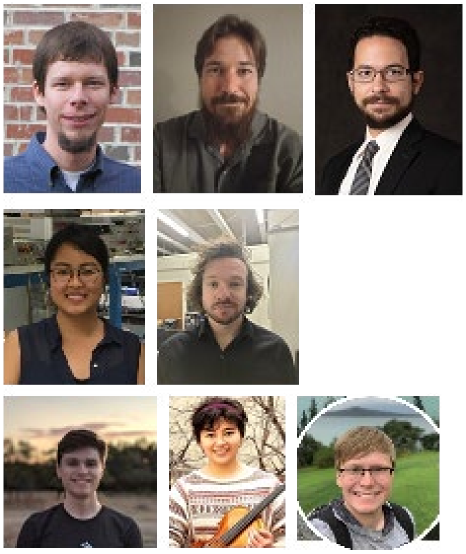

Figure 1. WCAPP Postdocs Bart Dunlap, Daniel Mayes, and Georges Jaar. Graduate Students Patty Cho, Kyle Swanson, Bryce Hobbs, Malia Kao, and Jackson White.

In addition to growth and evolution of experiments on Z, the increase in personnel has allowed WCAPP to expand to the use of other facilities, stimulated by the results of the original experiments. This has not been only at the largest scale, but the need to study magnetized plasmas at white dwarf stellar conditions has led to successful experiments on Zebra at the University of Nevada Reno. This gives students opportunities to carry out more shot experiments and provides more hands-on opportunities to carry out pulsed power experiments and be involved in most all phases of the work. This teaches and cross-trains scientists in a complementary way that is not possible on larger facilities.

A powerful example of the synergy created at the center with SNL is the work on stellar opacities appropriate to the problem of the depth of the solar convection zone. Solar models disagree on its position with helioseismic constraints from solar oscillations. Jim Bailey originally hypothesized that this problem might be partially resolved if the opacities of iron and oxygen are underestimated. Subsequent work showed that a part of the problem was the underestimation of iron opacity. It remains to answer the question, what is the opacity of the other major contributing element, oxygen?

Independently, the WCAPP team studying white dwarf stars wanted to study the radiative opacities beneath the convection zone in hot DQ (carbon-oxygen) white dwarf stars to understand their structure and evolution. These objects are thought to be white dwarf stars that have merged but with a combined mass too low to have become Type Ia Supernovae–the objects that led to the discovery of dark energy. These "failed supernovae" have much to teach us about stellar evolution and astrophysics: What does and does not explode in a Type Ia supernovae and why?

Bart Dunlap already had begun exploring gas cells with compositions appropriate to the DQ white dwarf surface layers, so the team could constrain the observations of their spectra used to constrain their mass and temperatures. Then they wanted to connect the improved understanding of the surface with the deep interior region where the opacity of oxygen may be highly significant.

You may ask, what does oxygen at the solar convection zone conditions have to do with oxygen at the base of a convection zone in a hot DQ white dwarf star? Especially, recalling that a white dwarf star is much more compact, about the size of the Earth and the mass of the Sun, the WD gravities are ten-thousand times stronger than solar type stars. It was only when Mike Montgomery began to model both solar stars and white dwarf stars and plotted their internal structure that they realized that the physical conditions at the base of the convection zone were almost the same as in a model of the sun as a white dwarf star. Shots were awarded on NIF to investigate oxygen opacity under white dwarf interior conditions. The NIF experiments are led by one of WCAPP's postdocs, Dan Mayes. He is involved directly in the Z oxygen opacity measurements as well. Now the team is in the fortunate position that two completely independent platforms and diagnostics are investigating oxygen opacity in a density-temperature domain so similar they can be intercompared across platforms. This will be tremendously useful in both applications and will improve confidence in the experiments in a way that will advance the national interest.

Nuclear Reaction Studies with Radioactive Ion Beams for Stewardship Science

Rutgers University ✦ PI: Dr. Jolie A. Cizewski (cizewski@rutgers.edu)

Nuclear Reaction Studies with radioactive ion beams for Stewardship Science (NRS4SS) was funded as of April 1, 2019 and builds on 16 years of previous Stewardship Science Academic Programs (SSAP) support. Central to NRS4SS is the synergistic collaboration with experimentalists Andrew Ratkiewicz and Nicholas Scielzo from Lawrence Livermore National Laboratory (LLNL), Steven Pain from Oak Ridge National Laboratory (ORNL), and theorists Jutta Escher and Gregory Potel (LLNL). The linchpin of this effort is the engagement of graduate students and postdoctoral scholars (postdocs) in all aspects of nuclear reaction studies with fission fragment beams from mounting experiments, to analysis and interpretation of the data, and dissemination of the results. Over the almost 19 years of SSAP support, seven Rutgers alumni have been placed at Los Alamos National Laboratory (LANL) and LLNL, including four who currently are staff members.

Research Highlight: Nuclear Reaction Studies with GODDESS for Stewardship Science

GODDESS – Gamma-array ORRUBA: Dual Detectors for Experimental Structure Studies[1] was realized under SSAP funding that enabled the development of the Oak Ridge Rutgers University Barrel Array (ORRUBA)—silicon-strip detectors of charged particles (Figure 1). GODDESS has enabled measurements of gamma rays in coincidence with charged particles to inform the synthesis of elements in stars and surrogates for neutron-induced reactions important for stewardship science. During the 2021 GODDESS campaign at ATLAS at Argonne National Laboratory (ANL), seven experiments were mounted, led by Rutgers, ORNL, LLNL, and university and international collaborators. Rutgers students and postdocs were critical to mounting the GODDESS system, taking data, and leading the analysis.

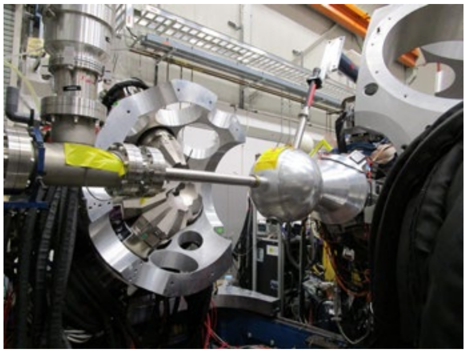

Figure 1. GODDESS in the 2021 campaign at the ATLAS accelerator at ANL where the GRETINA gamma-ray tracking array is coupled to ORRUBA and beam-like particles analyzed in a down-stream ionization chamber.

Figure 2. Watching the first acquisition of GODDESS 2021 data: Rutgers: Harry Sims (postdoc), Jolie Cizewski (PI) and Chad Ummel (SSGF): ORNL staff and Rutgers alumni: Steven Pain and Kelly Chipps. Photo courtesy of reference 5.

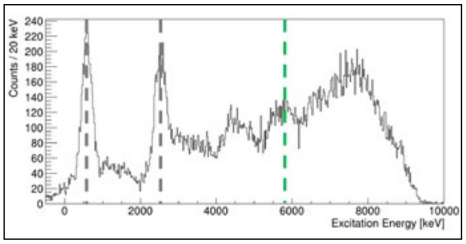

Figure 3. Preliminary proton spectrum from the 82Se(d,p) reaction as a function of excitation energy.[5] The neutron separation energy (green dashed) and important low-angular momentum (grey dashed) excitations are highlighted.

Almost all of the elements are synthesized in stars, including supernova explosions and mergers of neutron stars during which the heaviest elements are synthesized through the rapid neutron capture, r process. Ashes of these explosions are the observed stellar abundances of the elements. The atomic mass $A \approx 80$ peak in r-process abundance patterns presents a challenge to astrophysics because it probably reflects contributions from many astrophysical sites, including a “weak” r process that does not proceed to heavier nuclei. Some of these nuclei also are lighter fragments following fission of actinides. Surman and colleagues[2] analyzed the impact that uncertainties in nuclear physics data have in reproducing observed “weak” r-process abundances and highlighted the importance of data needs near the N=50 shell closure, in particular N=48 isotones. Near shell closures, neutron capture could proceed by two processes: direct capture and via the population and decay of a compound nucleus (CN). Direct capture depends upon excitation energies and spectroscopic properties of specific, low-angular momentum states, properties that readily are measured in a neutron-transfer (d,p) reaction. Away from the shell closures, the competition between direct and CN capture cannot be predicted. The Rutgers-LLNL collaboration validated the neutron transfer (d,pγ) reaction as a surrogate for neutron capture.[3] With GODDESS, both direct and CN capture cross sections as a function of effective neutron energy can be deduced in the same experiment.

In June 2021, Rutgers (PI Cizewski and postdoc Harry Sims) led the GODDESS measurement of the (d,pγ) reaction with ≈8.5 MeV/u beams of the stable N=48 isotone ^{82}Se (Figure 2). Although stable, there are only limited data on ^{82}Se(n,γ) cross sections, and the evaluations do not agree (EXFOR) in the neutron-energy region of interest for nucleosynthesis and stewardship science. The experiment was mounted with the same equipment and beam intensities that characterize RIB measurements, including analyzing the beam-like reaction products in a rate-limited ionization chamber. Preliminary spectroscopic properties of ^{83}Se states needed to inform DSD neutron capture have been deduced, and progress is being made in analyzing the particle-gamma coincidences to inform the ^{83}Se level scheme and extract the gamma-decay probabilities needed to inform neutron capture via the compound nucleus.

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

University of Nevada, Las Vegas ✦ PI: Dr. Pamela Burnley (pamela.burnley@unlv.edu)

Dr. Burnley's group at the University of Nevada Las Vegas (UNLV) (Figure 1) is investigating the deformation behavior of polycrystalline materials. The group is in the third year of their first Stewardship Science Academic Programs (SSAP) grant that supports three graduate students and two undergraduates. The group's primary focus is on high temperature, high pressure deformation of earth materials. However, their research spills over into metals, ceramics and organic compounds, and deformation at ambient conditions. Crystalline materials are, with few exceptions, anisotropic in their response to physical stimulus (e.g., changes in pressure, stress, strain rate, and temperature). Constrained within a polycrystalline material, individual crystalline domains experience varying boundary conditions according to the response of their neighbors as well as longer-range interactions. In addition, the grain boundaries themselves, although occupying an extremely small volume of material, can, in some cases, have significant effects on the overall strength of the aggregate. Taking all of this into account, it is no surprise that predicting overall material response is a challenge. A range of homogenization strategies (e.g., Voigt Reuss Hill average, self-consistent strategies) often are successfully utilized. However, there still are areas in which these strategies have less predictive power, in particular for understanding the development of shear localization. A powerful paradigm for understanding shear localization in granular materials is found in force chains. Burnley has proposed that this type of percolation-based description also may be useful for polycrystalline materials[1]. One of the group's projects is looking at how stress is distributed in loaded polycrystalline materials and how to quantify the stress distribution patterns. The second project looks at the role of grain boundaries as a function of pressure and temperature on nominally elastic behavior of polycrystalline materials.

Figure 1. Dr. Burnley's group Dr. Burnley's group in her high pressure lab working on re-assembling a piston-cylinder apparatus. From left to right: Taryn Traylor (PhD Student), Richard Panduro-Allanson (MS student), Genevieve Kidman (PhD student), and Sam Ofori (undergraduate).

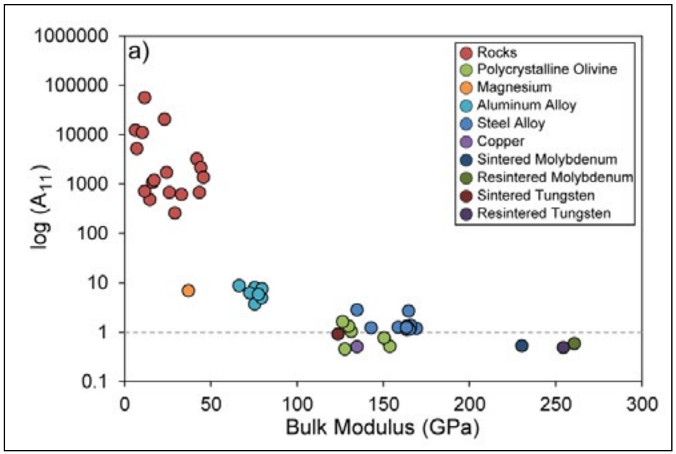

Figure 2. P-wave acoustoelastic constant (A_{11}) as a function of bulk modulus for polycrystalline olivine at high pressure as compared to rocks and metals at ambient conditions. See publication[2] for further details.

PhD student, Genevieve Kidman, has been working on mapping the stress distribution of slab-shaped samples of tigers-eye (fibrous quartz) using Raman spectroscopy. Raman spectral lines shift their positions as a function of pressure and, thus, can be utilized to measure the mean stress. The change in the Raman spectral lines is small for the stress levels achievable at ambient pressure, so Kidman developed a protocol for using plasma emission lines as internal standards to improve measurement precision. Her preliminary results indicate that the stress distribution within the loaded tigers-eye samples exceeds that predicted via elastic self-consistent modeling and that the spatial distribution of measured stresses does not correlate with the grain domains. These results are consistent with the stress distribution predicted by the presence of force chains. Genevieve just got back from a summer working on making similar measurements at Los Alamos National Laboratory using atomic force microscopy to observe Poisson's-ratio-related changes in topography of loaded tigers eye samples. She has been joined on the project by new MS student, Danny Panduro-Allanson, who is focusing on making finite element models of the samples.

PhD student, Taryn Traylor, is examining various measures of elasticity of polycrystalline materials at pressures between 1 and 10 GPa at temperatures up to 1,000 C using synchrotron X-ray diffraction in a multi-anvil apparatus. Burnley's group has observed, consistent with observations in metals, that polycrystalline materials are more compliant than the single crystal elasticity would predict and that this deviation is temperature dependent. Traylor also is making ultrasonic measurements of sound velocity during high pressure deformation measurements and has measured acoustoelastic constants of (Fe,Mg)$_2$SiO$_4$ (olivine)[2]. This is the first measurement of the acoustoelastic behavior of a silicate at high pressure. At high confining pressure the acoustoelastic behavior of olivine polycrystals is comparable to that of metals with a similar bulk moduli, in contrast to those of rocks where the bulk moduli is strongly decreased by the presence of cracks (Figure 2).

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Seeing through the Fission: Multi-modal Analyses of Actinides and Noble Gas Isotopes in Geological Samples

Washington University in St. Louis ✦ PI: Dr. Rita Parai (parai@wustl.edu); Authors: Scott Essenmacher and Chirag Vyas

The composition of Earth's atmosphere has evolved over time, and geological samples act as archives of ancient atmospheric compositions.[1] Noble gas isotopes are uniquely powerful tools with which to probe geological processes that have affected the atmosphere over time. However, interpretations of noble gas compositions measured in ancient rocks (up to 3.4 billion years old) are complicated by *in-situ* production of specific noble gas isotopes in the rocks by nuclear reactions over time. Since June 2019, the Stewardship Science Academic Alliances (SSAA) has supported collaborative work at Washington University in St. Louis, integrating distinct analytical techniques to address the effects of post-entrapment ingrowth and to better determine the trapped ancient atmospheric noble gas compositions. This work has been conducted by faculty members Rita Parai and David Fike, researchers Clive Jones and Julian Rodriguez, and students Mattison Barickman and Judy Zhang.

Volatile elements and compounds (such as water, carbon, nitrogen, and the noble gases) have been transported between the Earth's deep interior and the atmosphere over time in association with volcanism and plate tectonics.[2] Atmospheric loss to space also has affected the atmospheric composition over time.[1] Constraints on the isotopic compositions of atmospheric noble gases provide insights into the timing and rates of volatile transport over Earth history.

The aim of the work is to harness multiple modes of geochemical analysis to rigorously correct for post-entrapment production of noble gas isotopes in siliceous geological samples, known as cherts, to better elucidate how the trapped ancient atmospheric compositions have changed over time. This work is important to stockpile stewardship, because it trains the next-generation of scientists in multiple, advanced analytical techniques (including secondary ion mass spectrometry, X-ray adsorption spectroscopy, and high-precision noble gas isotope ratio mass spectrometry) and requires the integration and interpretation of disparate datasets to address a complex problem.

The abundances of trace elements (uranium, thorium, barium, tellurium) have been characterized *in situ* by secondary ion mass spectrometry (SIMS) using the Cameca ims 7f/geo run by David Fike at Washington University. Graduate student, Matt Barickman, prepared sets of chert samples for analysis with a range of ages from a few hundred million years to 3.4 billion years old (Figure 1). Ion images are taken to map out abundances of isotopes that are important to the study: for example, spontaneous fission of ^{238}U generates specific isotopes of Xe over time, so sub-samples with low ^{238}U abundances are sought to minimize post-entrapment fissiogenic Xe ingrowth.

Paired chips of the same samples analyzed by SIMS are being analyzed for noble gas isotope ratios using the facilities run by Rita Parai. Gases are extracted from chert samples by crushing under vacuum using a hydraulic ram, and released gases are purified for analysis using getter pumps. Neon, argon, krypton, and xenon are trapped using cryogenic cold trap systems and are sequentially released to a low-volume, high-sensitivity gas source isotope ratio mass spectrometer specifically designed for high precision noble gas isotope analysis. The cryogenic traps required modification to resolve a design issue that was preventing satisfactory separation of noble gases for analysis. Junior participants carried out modifications to thermal anchors within these systems and successfully addressed this challenge (Figure 2), gaining a deeper knowledge of how these systems work and experience with trouble-shooting instrumentation. Having resolved the issue, high-precision noble gas isotopic analyses are underway.

References

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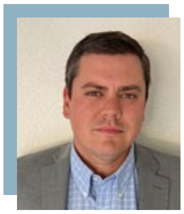
Figure 1. Fragments of a 3.4 billion year old chert sample are cleaned prior to analysis.

Figure 2. (From left to right) Students Judy Zhang, Matt Barickman, and Julian Rodriguez modifying a cryogenic trap to improve separation of noble gases for mass spectrometric analysis.

Jonathan King, National Nuclear Security Administration, Livermore Field Office (jonathan.king@nnsa.doe.gov)
Years at LFO: 2019-Present, **Degree:** PhD, Nuclear Chemistry ✦ **SSAA Program:** 2012-2018, Oregon State University



I always have had a keen interest in the chemistry, physics, and engineering underpinning U.S. nuclear weapons. Through the support of the Stewardship Science Academic Alliances (SSAA) program, I was able to complete my PhD in Nuclear Chemistry at Oregon State University (OSU) under Dr. Walter Loveland. Funded by the SSAA, my dissertation focused on measuring the fast neutron induced fission of ^{232}Th, which ultimately propelled me into my current position within the Nuclear Security Enterprise (NSE).

While continuing work on my PhD in 2016, I accepted a position with the Department of Energy/National Nuclear Security Administration (DOE/NNSA) Graduate Fellowship Program (NGFP) in Washington, DC working in the DOE/NNSA's Office of Technology Maturation. During that time, I had the privilege of visiting every site within the NSE, experiencing everything from watching a Minuteman III launch at Vandenberg Air Force Base to observing nuclear weapon assembly activities at Pantex. This unique opportunity afforded me a comprehensive view of DOE/NNSA facilities and capabilities that I will carry throughout my professional career.

At the conclusion of the NGFP fellowship in 2017, I was offered a position in the NNSA as a federal employee. I went on to lead several programs at DOE/NNSA headquarters that sought to advance U.S. nuclear weapon capabilities and manufacturing. One personal highlight during this period was successfully securing initial funding for DOE/NNSA's High Operational Tempo Sounding rocket (HOT Shot) program. HOT Shot is a research program that launches sounding rockets into space to test future nuclear weapon components and manufacturing technologies in relevant launch environments as an avenue for technology maturation (Figure 1).

Figure 1. HOT Shot 1 sounding rocket launch out of the Pacific Missile Range Facility, which King secured funding for.

I completed my PhD remotely in 2018 while working full time for the DOE/NNSA. Though it was an enormous challenge, I was able to complete my degree thanks to the constant support from my thesis advisor and my DOE/NNSA management team.

In 2019 I took a promotion out to DOE/NNSA's Livermore Field Office (LFO), as a Defense Programs (DP) liaison, working with a small team to oversee all nuclear weapon development activities at Lawrence Livermore National Laboratory (LLNL) (Figure 2). Transitioning from DOE/NNSA headquarters to the field has increased my exposure to the technical work, facilities, and capabilities of one of our nuclear physics design agencies, LLNL. I'm continually impressed by the extremely high caliber of people working for our Management and Operating (M&O) partners, and as a DP liaison I do everything that I can to enable their vital national security work.

> *“SSAA's support of my PhD was pivotal in my ability to pursue a career in nuclear weapon design agency oversight, and for that I am eternally grateful.”*

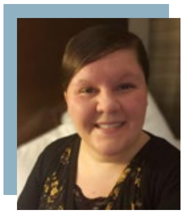
Figure 2. King oversees the LLNL stockpile stewardship activities that ensure the continued reliability of the Air Launched Cruise Missile (ALCM) warhead, the W80-1.

In conjunction with my DP liaison role, I recently was given the opportunity to become a Federal Team Lead with DOE/NNSA's Radiological Assistance Program (RAP), which is an organization within the Nuclear Emergency Support Team (NEST). This is one of the teams that is prepared to rapidly deploy to any radiological incident in the United States, up to and including the detonation of a nuclear weapon. Our team is responsible for California, Nevada, Hawaii, and the U.S. Pacific Territories. Though I'm still a new member of the team, being a part of this emergency response program has provided yet another view of the impressive capabilities and important missions of the DOE/NNSA.

SSAA's support of my PhD was pivotal in my ability to pursue a career in nuclear weapon design agency oversight, and for that I am eternally grateful. I am proud to spend my career advancing the security of the United States, and I owe that opportunity in some part to the SSAA.

Andrea Richard, Lawrence Livermore National Laboratory (richard10@llnl.gov)

Years at LLNL: April 2021-Present, **Degree:** PhD, Nuclear Physics ✦ **SSAA Program:** 2012-2018, Ohio University (Graduate Student); 2019-2021, Michigan State University (Postdoctoral Fellow)



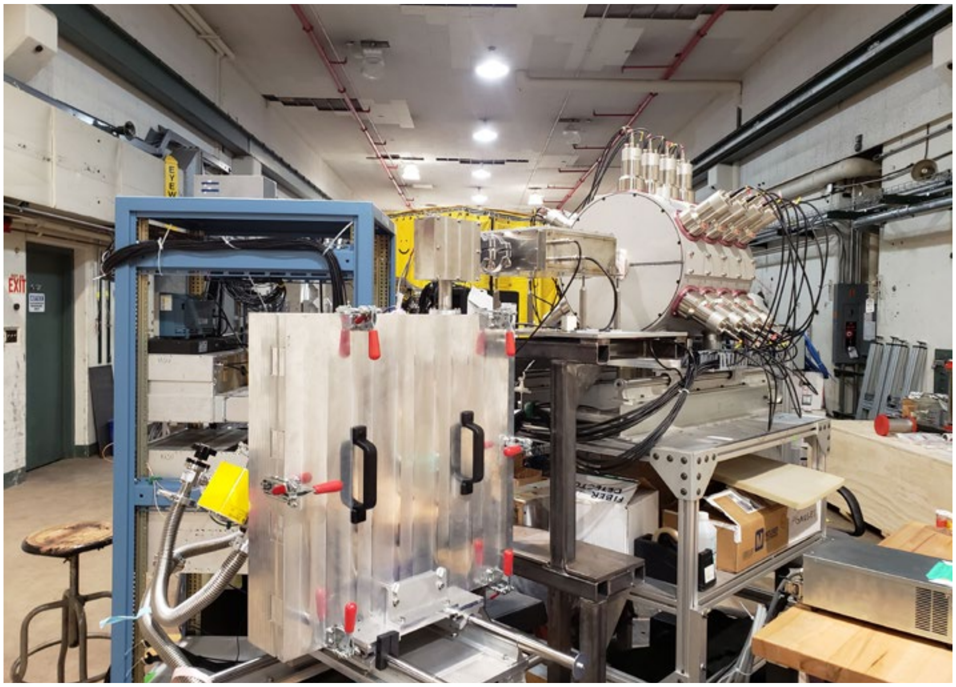


Figure 1. The SuNTAN detector is currently being utilized for an experimental campaign at ANL's CARIBU facility, where the β-Oslo method is being used to experimentally constrain neutron-capture cross sections related to stockpile stewardship and nuclear astrophysics. In the future, the SuNTAN detector and β-Oslo technique will continue to be used at facilities such as ANL and the upcoming Facility for Rare Isotope Beams (FRIB).

Support from the Stewardship Science Academic Alliances (SSAA) program was instrumental in guiding my career. It allowed me to collaborate with scientists from various universities and national laboratories and to develop research connections that led me to my present position at Lawrence Livermore National Laboratory (LLNL). Throughout my research work, the need for detailed nuclear data has become apparent. Vital quantities such as neutron-capture cross sections and rates, β-decay half-lives, and masses inform our understanding of reaction networks for astrophysics and applications that can address the Nation's needs.

My first exposure to the SSAA program was as a Master of Science (MS) student at Ohio University where I worked on neutron time-of-flight spectroscopy at the Edwards Accelerator Laboratory (EAL). During my MS thesis, we measured the deuteron breakup reaction to better understand the low-energy neutrons coming from the $^{2}\text{H}(d,n)$ reaction which is used for the active interrogation of hidden fissile materials and other applications. While a graduate student at Ohio University, I was involved in the planning and execution of experiments for many groups interested in using the neutron capabilities at the EAL including groups from LLNL and Los Alamos National Laboratory. During my dissertation at Ohio University, I worked on basic science research using radioactive beam studies in the A=33 region at the National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University (MSU) in collaboration with scientists at Lawrence Berkeley National Laboratory. Each of these projects highlighted the fundamental need for nuclear data in all realms of nuclear science, from basic research to applications in medicine and nuclear security.

After completing my PhD in 2018, I joined the NSCL as a postdoctoral fellow. This was made possible due, in part, to support from the SSAA and connections that were made during my dissertation work. As a postdoctoral fellow at the NSCL, I used an indirect technique known as the β-Oslo method to constrain neutron-capture reactions on short-lived nuclei that are important for astrophysics and stockpile stewardship. This method relies on the β-decay of radioactive isotopes to populate the compound nucleus of interest and utilizes total absorption spectroscopy coupled with statistical reaction techniques to extract the nuclear level density and gamma-ray strength function. These quantities are then used as inputs into Hauser-Feshbach calculations, and experimentally constrained (n,γ) cross sections are obtained. While I was a postdoc at MSU, I participated in countless experiments at the NSCL as well as at Argonne National Laboratory (ANL), collaborating with scientists from various universities and national labs. Figure 1 shows the detector setup for a β-Oslo campaign that currently is ongoing at ANL using the CARIBU (CAlifornium Rare Isotope Breeder Upgrade) facility and the SuNTAN detector (Summing NaI + Tape system for Active Nuclei).

Early in 2021, I joined LLNL as a postdoctoral researcher where I am utilizing another indirect technique to constrain neutron-capture cross sections. This reaction-based indirect technique is known as the surrogate-reaction method and uses high-resolution gamma-ray spectroscopy and (d,p) reactions as a surrogate for the (n,γ) reaction. It has been applied for fission fragments and for reactions relevant for astrophysics. By applying and understanding both indirect methods, we can benchmark the available neutron-capture techniques, utilize the mechanism that best fits the intended scientific goals and capabilities of different experimental facilities, and better understand their systematic variations.

Access to even more exotic nuclei will become available soon due to the opening of the Facility for Rare Isotope Beams (FRIB), which will be the leading radioactive beam facility in the US. This facility will provide even more opportunities to study nuclei that have never been observed before and to address questions related to nuclear structure, astrophysics, and how radioactive isotopes can benefit society via medical and security applications.

Manolo E. Sherrill, Los Alamos National Laboratory (manolo@lanl.gov)
Years at LANL: 2003-Present **Degree:** PhD, Physics ✦ **SSAA Program:** 1999-2003, University of Nevada, Reno

Since 2020, I have been the Advanced Simulation and Computing (ASC) Program Manager of the Physics and Engineering Models (PEM) Program at Los Alamos National Laboratory (LANL). LANL's PEM program develops many of the material models used by the weapon design and safety modeling communities, as well as the nuclear non-proliferation community. These models and their corresponding projects span a wide range of topical areas: high explosives, equation-of-state (EOS), material strength and damage, atomic and molecular opacities, nuclear data, shock-generated ejecta, and turbulence. Two newer projects, Threat Reduction and Enabling Manufacturing, apply the classical subject areas above to the nuclear non-proliferation and plutonium pit manufacturing communities. My responsibility as the PEM Program Manager is to align research activities in the above topical project areas to laboratory and Department of Energy/National Nuclear Security Administration (DOE/NNSA) priorities.

While I was pursuing my PhD at the University of Nevada, Reno under Professor Roberto C. Mancini, I had the privilege of participating in the Stewardship Science Academic Alliances (SSAA) program. During this time, I had the opportunity to interact with several LANL and Sandia National Laboratories (SNL) scientists. Although my researched ultimately focused on spectroscopic modeling of a laser ablation experiment performed at SNL by James Bailey (Figure 1), I had an opportunity early on to perform radiation-hydrodynamic simulations of laser ablated graphite targets. This was my first experience following fluid element trajectories across a realistic EOS through various phase transitions, and the first time that I observed the pinning of trajectories to the phase boundaries—a phenomenon that occurs when lasers of low fluence are unable to provide the energy needed for the latent heat of a transition. Interestingly, I would later encounter this phenomenon in high-explosive-driven metals. I encountered many such phenomena during my graduate education and training that I later observed throughout my career at LANL.

Through the SSAA, I interacted with LANL's EOS team and the atomic physics team, and I eventually chose LANL for my postdoctoral research position through our collaboration with noted atomic physicists, Robert D. Cowan and Joseph Abdallah Jr. During my PhD, I implemented a capability into the LANL suite of atomic physics codes for use in my research that allowed accurate modeling of neutral and near-neutral mid-Z atomic structure, such as silver, necessary for modeling the Sandia ablation experiments (Figure 1). I became a LANL staff scientist in 2006, at which time I began developing models for non-local thermodynamic equilibrium (NLTE) models for the high-Z elements. In 2009, I was the LANL lead for the LANL/Sandia collaboration on opacity modeling and associated experiments. A year later, I began the development of a self-consistent radiation and atomic physics capability at LANL (Figure 2). This capability reveals the complex behavior observed in plasma spectroscopy of radiatively driven experiments. A few years later, I began massively parallel three-dimensional, radiation-hydrodynamic simulations of the Sandia Z-pinch dynamic hohlraum. My final technical area has been in the design of novel weapon. For all of these professional activities, I have relied on the experiences I gained during my graduate education and my numerous interactions with the DOE/NNSA laboratories and my time in the SSAA.

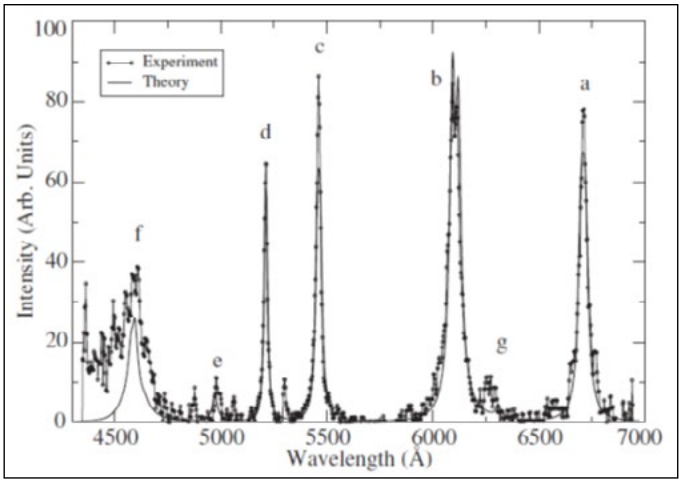


Figure 1. Experimental and theoretical spectra of a lithium-silver ablation plasma. Spectroscopic characterization revealed a plasma with varying density and temperature profiles: Te=[0.7, 1.8, 1.8, 0.7] eV and Na=[1.0, 2.0, 2.0, 1.0]x10^{17} cm−3 respectively. James Bailey at Sandia performed the experiment. Theoretical modeling by Manolo Sherrill (PhD dissertation) and Roberto Mancini (dissertation advisor). Spectral features a, b, and e, arise solely from Li while lines c, d, and f arise solely from Ag.

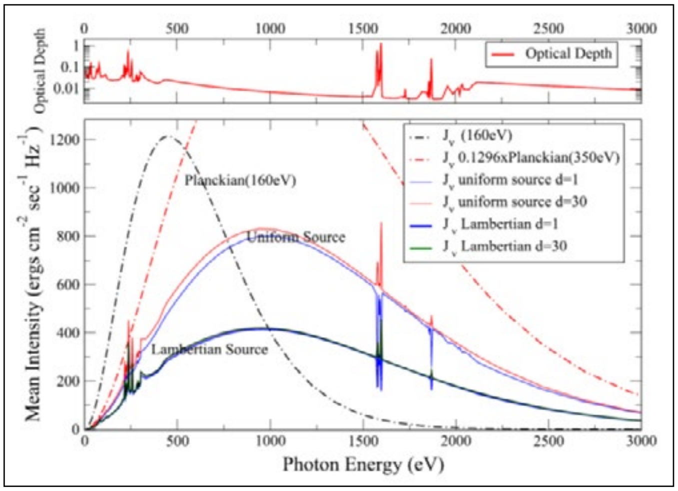


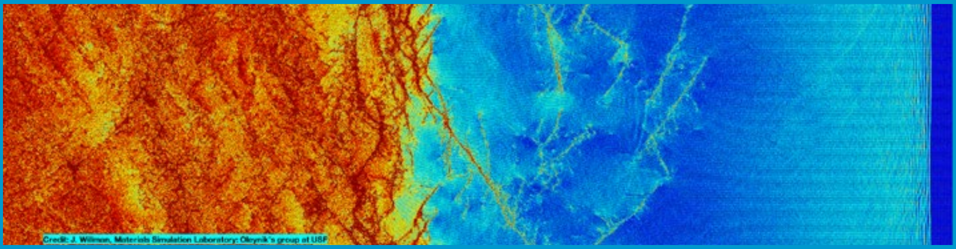
Figure 2. Much like the Sun where deep layers of the stellar atmosphere are near equilibrium while the outer layers near the surface are strongly out of equilibrium, so too is the behavior of a single-sided radiatively driven laboratory plasma. The lower plot illustrates the spectra observed from two different types of radiative drives, uniform and Lambertian. In either case, the deep layers (d=30) of this aluminum plasma reveal emission lines while the shallow layers (d=1) exhibit absorption lines and are highly out of equilibrium. This difference is the consequence of the outer layers trapping radiation and sending it back toward the deeper layers while the surface layer only sees an open sky. Self-consistent simulations such as these allow for the detailed characterization of laboratory plasma.

Students

Stewardship Science Academic Alliances

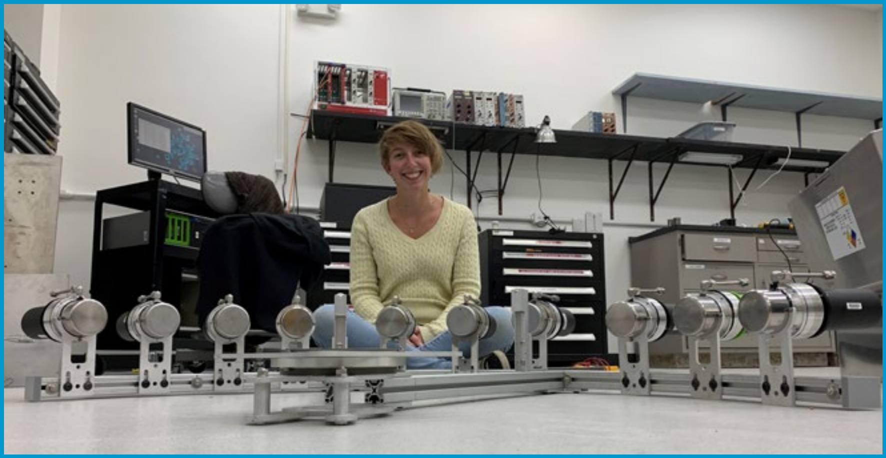
Ian Cox (front) helping to construct VANDLE detector modules for FRIB Decay Station Initiator. (p. 24)

Ashley Hastings working inside University of Notre Dame Actinide Center of Excellence dispersible plutonium glovebox for the preparation of a plutonium MOF sample. About 40 mg of the pink powder was loaded into a tube for a nitrogen sorption isotherm experiment. (p. 24)



Credit: J. Willman, Materials Simulation Laboratory: Oleynik's group at USF

This figure displays the complex nature of inelastic deformations in a shock compressed diamond. The image consists of 2 billion atoms within a 1 µm-thick diamond sample, they are colored by atomic potential energy (uncompressed, lowest energy – dark blue; highly compressed, the highest energy – bright orange/yellow). Jonathan Willman (p. 26)

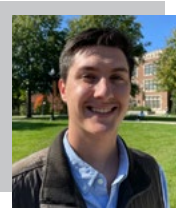


Rebecca Toomey with 10 deuterated liquid scintillator ODeSA neutron detectors. These detectors were mounted at the University of Notre Dame to measure the $^{18}O(\alpha,n)$ reaction that is important for nuclear non-proliferation and applications in geophysics and astrophysics. (p. 26)

Kyle Swanson configuring vertical laser interferometry diagnostics for electron density measurements of photoionized supersonic gas jets on the Zebra pulsed-power accelerator. (p. 25)

Ian Cox (icox2@vols.utk.edu)

Degree in Progress: PhD, Nuclear Physics, University of Tennessee, Knoxville ✦ **Advisor:** Dr. Robert Grzywacz ✦ **SSAA:** 2020-Present



Research Topic

Decay Studies of Rare Isotopes using Novel, Fast, Segmented Scintillators

Research Responsibilities

I work in a low-energy nuclear physics collaboration, studying the decays of exotic nuclei. Experiments to study these decays are conducted at rare isotope beam facilities worldwide, such as the Radioactive Isotope Beam Factory (RIBF) at RIKEN and the Facility for Rare Isotope Beams (FRIB) at Michigan State University (MSU). My work focuses on developing a detector that can stop the radioactive ions and measure their subsequent decays. Measurements of decays provide insight into nuclear structure and also can help to learn about astrophysical processes, such as the r-process. This implantation detector consists of a multi-anode photomultiplier tube coupled to a fast-response, segmented scintillator, which allows for time and spatial correlations within the detector. Generally, it is used alongside other detector systems, such as the Versatile Array of Neutron Detectors at Low Energy (VANDLE) neutron detector array or other gamma-ray detectors, to measure decay chains due to the fast-timing capabilities of the detector. The detector segmentation is critical to utilizing this detector with cocktail beams typically used in fragmentation facilities and to enable the study of decays of very exotic isotopes. At FRIB it will be utilized in the FRIB Decay Station Initiator system for neutron spectroscopy. At RIBF RIKEN, it will be used for decays near 100 Sn. My research responsibilities are to optimize the detector performance and to carry out successful experiments.

Benefits of SSAA

One of the main benefits of the Stewardship Science Academic Alliances (SSAA) is the ability to meet other researchers in fields that pertain to my research. As someone who works with scintillators and multi-anode photomultiplier tubes, it has been beneficial to see how they are developed or used for other experiments. While restrictions have limited the ability for in-person conferences, the accessibility of online conferences and other seminars has greatly helped push forward research and has allowed for a better understanding of what others in the field are working towards.

What Students Considering SSAA Should Know

For new students, SSAA is a great resource for meeting other researchers, many of whom are in a similar field. By meeting and making connections with researchers from other institutions, you can increase the ability to get a postdoctoral position after graduating. Overall, funding from the SSAA has helped me to engage in exciting research and has given me the opportunity to travel for experiments.

Ashley Hastings (ahastin1@nd.edu)

Degree in Progress: PhD, Actinide Chemistry, University of Notre Dame ✦ **Advisor:** Dr. Amy E. Hixon ✦ **SSAA:** 2018-Present

Research Topic

Frontiers in Actinide Metal–Organic Framework Chemistry

Research Responsibilities

My research pushes the limits of actinide-based metal–organic frameworks (MOFs) with respect to metal selection, metal-ligand coordination, and stability in high radiation fields. MOFs are a class of hybrid materials known for their diverse architectures, which yield high surface areas and other favorable characteristics. Key opportunities with respect to rational design and structural tunability allow for targeted functionalities (e.g., gas storage, sensing, catalysis, and more). Actinide-based MOFs, however, offer distinct opportunities from transition metal-based MOFs because of their radioactivity and the fascinating chemistry of 5*f*- and 6*d*- orbitals. More specifically, I have synthesized the first plutonium-based MOF, Pu-UiO-66, provided proof-of-concept work that actinides may coordinate to softer N-donor linkers in addition to the usual carboxylate-based ligands utilized heavily thus far, and systematically studied the role of metal selection in the radiation stability of isostructural MOFs.

Benefits of SSAA

Funding from the Stewardship Science Academic Programs (SSAP) has equipped my lab with a wide range of instrumentation. As my work involves the handling of radioactive materials, it is helpful, and often essential, that access to the analytical instruments I need is available in my immediate, radiologically-approved facility. This has allowed me to play an integral role in my own sample preparation, data collection, and data interpretation. Additionally, we have the opportunity on select instruments to have a greater role of responsibility with general maintenance, trouble shooting, and training other lab members. I have gained a range of experience and expertise on X-ray-based, spectroscopic, and many other characterization techniques.

New Contacts, New Opportunities

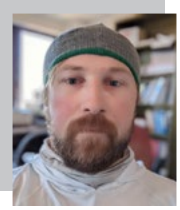
The SSAP grant that resulted in the Actinide Center of Excellence (ACE) founded a well-crafted team of multi-institutional collaborators with individual niches of expertise. My work, in particular, benefits greatly from the synergy of the center. Our collaborators at Northwestern University (NU) have provided invaluable discussion, context, and even provision of starting material for some of my projects. While my background and immediate surroundings are actinide chemistry, my NU collaborators corroborate my findings at the forefront of emerging developments in the MOF community. I also greatly leverage the assistance of my computational collaborators at the University of Chicago and University of Minnesota. These collaborations augment our understanding of complex systems and enable us to report well-developed stories. My familiarization with ACE personnel through virtual meetings and other engagements enabled me to quickly reach out for assistance when necessary. The advantage is mutual, as I have similarly been able to assist other ACE students in their work.

Christopher D. Noble (cdnoble@wisc.edu)

Degree in Progress: PhD, Engineering Physics, University of Wisconsin-Madison ✦ **Advisor:** Dr. Ricarro Bonazza ✦ **SSAA:** 2015-Present

Research Topic

Shock-Driven, Turbulent Mixing



Research Responsibilities

I study the Richtmyer-Meshkov instability using the Wisconsin Shock Tube Laboratory's 9 m tall, vertically firing shock tube, using high-speed, planar, laser-induced, fluorescence and particle image velocimetry. I am responsible for the design, setup, execution, and analysis of experiments, as well as the preparation of the first drafts of papers and presentations. I have presented this work at a number of international conferences. I also aid other graduate students in the lab with experiment design, setting up optics, camera timings, and laser actuation for their work, using experience from running my own experiments.

Benefits of SSAA

The Stewardship Science Academic Programs (SSAP) has allowed me the ability to perform exciting novel experiments, to attend intellectually stimulating summer schools, and to present at international conferences, giving me access to a broad range of ideas and connections.

New Contacts, New Opportunities

The SSAP program made it possible for me to travel to Marseille, France to present at the international workshop on the physics of compressible turbulent mixing (IWPCTM). This was my first experience presenting a talk. SSAP had provided me with two opportunities that were invaluable in preparing me. First, an opportunity to present a poster along with another graduate student at the Department of Energy/National Nuclear Security Administration (DOE/NNSA) SSAP symposium in Naperville, IL. This was the first time we would meet fellow graduate students from other labs around the country who work in our field and allowed us to gain experience fielding questions about our work. Second, it gave me a chance to attend the American Physical Society - Division of Fluid Dynamics conference in Denver, Colorado, giving me the freedom to explore the conference and to network.

With the experiences I was afforded, I was able to make the most of the talk at IWPCTM to connect with some great people working in our field. This allowed me connections I could call upon further along in my PhD research to ask for advice or to potentially collaborate.

The SSAP also indirectly has helped me. Another graduate student in our group was able to participate in two internships at Lawrence Livermore National Laboratory, allowing them access to computing resources and access to the Miranda fluid dynamics simulation software. Computations they have performed have provided an extremely useful database to test data analysis algorithms and to investigate the parameter space to help hone our expectations and understanding of experimental results.

Kyle James Swanson (kswanson.unr@gmail.com)

Degree in Progress: PhD, Laboratory Astrophysics, University of Nevada, Reno ✦ **Advisor:** Dr. V.V. Ivanov and R.C. Mancini ✦ **SSAA:** 2016-Present

Research Topic

Laboratory Photoionized Plasmas Relevant for Astrophysics (X-ray Binary, Warm Absorbers, Active Galactic Nuclei)

Research Responsibilities

As a graduate student, I wear many hats, resulting in diverse responsibilities, duties, and learning opportunities. For experiments, I either lead or support the experimental design. I am responsible for all aspects of the experiment set-up such as sample/target and hardware preparation. During experiments, I configure and field the diagnostics responsible for the observations made. Afterward, I perform post-experiment assessment and cleanup. In parallel, I also develop the code necessary for data processing and analysis.

Benefits of SSAA

The Stewardship Science Academic Alliances program has provided opportunities and experiences unlike anything typically possible for a graduate student. The main impact has been my experience in laboratories normally only accessible after one has graduated. This leads to the primary benefit I have gained—the connections made with world renowned scientists and the other students.

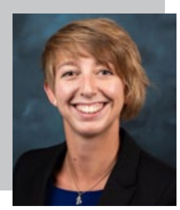
National Laboratory Experience

I have had the opportunity to conduct my PhD research in the field of high-energy density laboratory astrophysics, specifically focused on photoionized plasmas. Such plasmas are found in highly energetic astrophysical environments such as those around accretion powered objects like blackholes. These celestial engines generate high-intensity broadband UV and X-ray radiation which heats and ionizes the surrounding gas into a photoionized plasma. Through laboratory studies, we improve our interpretation and understanding of these astrophysical phenomena. Astrophysically relevant laboratory photoionized plasmas require large-scale pulsed-power generators. This placed me at the helm of two powerful machines: Zebra a 1MA pulsed-power generator at the University of Nevada, Reno and the Z machine, the world's most powerful X-ray source, at Sandia National Laboratories. I cut my teeth on Zebra, helping develop new scientific platforms for photoionized gas jets and mega Gauss magnetized plasmas. I gained experience implementing a plethora of laser and X-ray diagnostics, ranging from multi-color interferometry to crystal and diffraction grating spectroscopy. Once I was given the keys to the gas cell platform on Z. I took the opportunity to implement a new laser diagnostic, allowing time-resolved electron density measurements. Z is impressive and what was just as impactful is the team effort. It sharpens and focuses the ideas of each team member which is powerful and effects all stages of the scientific effort. The skills, techniques, and methodologies I developed and cultivated from my time on Zebra and Z have been priceless, affording me new experiences and perspectives about what can be done, how powerful a team can be, and what it means to contribute, culminating in an immensely rich and productive experience.

Rebecca Toomey (rebecca.toomey@rutgers.edu)

Degree in Progress: PhD, Nuclear Physics, Rutgers University ✦ **Advisor:** Prof. Jolie Cizewski ✦ **SSAA:** 2016-Present

Research Topic



High-resolution Measurement of the $^{18}O(\alpha,n)^{21}Ne$ Reaction Utilizing the Spectrum Unfolding Method of Neutron Spectroscopy

Research Responsibilities

The $^{18}O(\alpha,n)^{21}Ne$ reaction has been identified as a reaction of interest in many different sub-fields of nuclear physics and its applications. For the verification of nuclear material, $^{18}O(\alpha,n)^{21}Ne$ is a dominant neutron-producing reaction in nuclear fuels. Neutron source calculations for nuclear material rely on nuclear data. A crucial ingredient of these calculations are partial cross sections and branching ratios, which have not been measured previously. As such, I led the effort to measure the $^{18}O(\alpha,n)^{21}Ne$ reaction using the Oak Ridge National Laboratory (ORNL) Deuterated Spectroscopic Array (ODeSA), and I am leading the analysis of this data set. I built five of the ten deuterated liquid scintillator ODeSA neutron detectors and participated in the full characterization of the array at Ohio University and the Los Alamos Neutron Science Center (LANSCE) at Los Alamos National Laboratory (LANL).

Benefits of SSAA

My journey as a researcher has been greatly impacted by my involvement with the Stewardship Science Academic Alliances (SSAA). As an undergraduate, SSAA funding allowed me the opportunity to participate in cutting-edge research and to travel to meetings and conferences. It showed me the diversity and quality of research that the Department of Energy/National Nuclear Security Administration (DOE/NNSA) sponsors, and these opportunities ultimately spurred me on to pursue a PhD in Nuclear Physics. As a PhD student, I have learned how the SSAA is able to foster collaboration between a variety of fields. For example, at the 2020 SSAP Symposium while discussing my research on the $^{18}O(\alpha,n)^{21}Ne$ reaction with geophysics researchers from Washington University, I discovered that my measurement has direct implications for their research into the dynamics of Earth's mantle, providing me with an additional motivation for my measurement. Without the SSAA my career would not be where it is today.

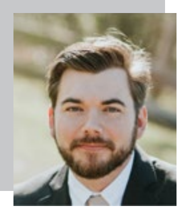
What Students Considering SSAA Should Know

My research has been shaped by opportunities I have had at the DOE/NNSA national laboratories. Funding from the SSAP has allowed for me to attend workshops at LANL and at Lawrence Livermore National Laboratory (LLNL), which were unique opportunities for me to discuss research and to tour the facilities. Discussion breeds collaboration. A prime example: further characterization of ODeSA is currently underway at the LANSCE facility at LANL. In addition, with my involvement in the construction and utilization of ODeSA, I have been in permanent residence at ORNL working with my collaborators and preparing for experiments.

Jonathan Willman (jwillma2@usf.edu)

Degree in Progress: PhD, Applied Physics, University of South Florida ✦ **Advisor:** Dr. Ivan Oleynik ✦ **SSAA:** 2017-Present

Research Topic



Atomistic Molecular Dynamics Simulations of Dynamically-compressed Materials using Machine-learning Interatomic Potentials

Research Responsibilities

As a member of Dr. Ivan Oleynik's group, I am investigating carbon at extreme conditions created by strong shock compression. Studies of carbon at extreme conditions are of great fundamental and practical importance for developing models of carbon-rich exoplanets as well as achieving ignition in inertial confinement fusion experiments where diamond shells are used as fuel-containing ablation capsules. I have developed a machine-learning interatomic potential for carbon, which is now being applied to simulate diamond shock compression at experimental ns and μm time and length scales using DOE leadership-class supercomputer Summit, one of the fastest computers in the world. Among several highlights from our work are fundamental atomic-scale understanding of anomalous strength and inelastic deformations in shock-compressed diamond.

Benefits of SSAA

I have had an exceptional opportunity to collaborate with world-class scientists from Sandia National Laboratories (SNL) and LLNL in several joint theory/simulation and experimental projects. In particular, I am fortunate to work with Drs. Aidan Thompson and Mitchell Wood from SNL, the inventors of Spectral Neighbor Analysis Potential, who introduced me to the frontiers of materials modeling—applications of machine learning to devise quantum-accurate description of interatomic interactions. I also contribute to several ongoing collaborative efforts within National Ignition Facility (NIF) Discovery Science (Drs. Jon Eggert and Marius Millot, LLNL) and Z Fundamental Science (Patricia Kalita and Tom Ao, SNL) programs. Our contribution is to provide theoretical guidance to experiments at the leading dynamic compression facilities.

National Laboratory Experience

I was fortunate to spend several weeks in January and February of 2019 at SNL working with Drs. Thompson and Wood to learn the fundamentals of machine learning potential development. Although the pandemic severely affected in-person interactions, I tremendously benefitted from day-to-day virtual communications with our SNL collaborators. Our team, which consisted of researchers from USF (myself, K. Nguyen Cong and I. Oleynik), SNL (A. Thompson, M. Wood and S. Moore), NERSC/LBL (R. Gayatri) and NVIDIA (E. Weinberg) performed a billion atom simulation of carbon at extreme conditions on Summit and broke the world record of fastest quantum accurate molecular dynamics simulation. Our groundbreaking results earned a finalist nomination for the prestigious Gordon Bell Prize, the equivalent of Nobel prize in supercomputing.

High Energy Density Laboratory Plasmas Program

Zeeman Effect in Hydrogen at 2-3 MG Magnetic Fields

University of Nevada, Reno ✦ PI: Dr. V.V. Ivanov (ivanov@unr.edu)

Strong magnetic fields dramatically change properties of plasma. Studies of magnetized plasmas are relevant to many fields of basic and applied plasma physics as well as to astrophysics. Strong magnetic fields improve conditions for inertial confinement fusion and change the dynamics of plasma expansion and the development of instabilities.

For a long time, a linear Zeeman effect was the one spectroscopic feature of matter in the magnetic field. The linear Zeeman effect was used for measurements of the magnetic fields in laboratory and stellar plasmas. The quadratic Zeeman effect should appear in strong fields >2 MG (million Gauss). For the first time, we investigated the linear and quadratic Zeeman effects in a laboratory plasma at magnetic fields of 2-3 MG. These studies help to find a signature of the quadratic Zeeman effect in spectra of White Dwarf stars where magnetic fields reach strengths of 1-200 MG.

We used an experimental platform developed at the University of Nevada, Reno. The Zebra pulsed power machine generates 2-4 MG magnetic fields from rod loads. A small droplet of CH oil on the load was the source of the hydrogen. Radiation of the load with a temperature of 0.5-0.7 eV backlit exited hydrogen atoms in the oil droplet. A rod load and a cross-section are shown in Figure 1(a,b). A load diameter and material varied to reach the maximum of the B-field before the total evaporation of the load. Spectra of absorption hydrogen Balmer lines at 656 nm and 486 nm were studied. Typically, these absorption lines are seen in stellar atmospheres. Figure 1(c) shows a Zeeman triplet in aluminum loads with a 3.9 nm split. The split corresponds the magnetic field of 1.9-2.1 MG. These fields are in agreement with measurements of the magnetic field by Faraday rotation and B-dot diagnostics. A Cu load 0.9 mm in diameter allow measurements near the maximum of the current pulse. The Zeeman split of 6.2 nm corresponds to a B-field of 3 MG, shown in Figure 1(d).

The quadratic Zeeman effect shifts the central line of the Zeeman triplet to shorter wavelengths. The shift is more pronounced in the H-beta transition as seen in Figure 1(e). The experimental point from 3 shots with aluminum loads presents the first measurement of the quadratic shift at B=2 MG. Additional measurements of the quadratic Zeeman shift in H-alpha and H-beta lines will be performed with copper, gold, and silver loads in the range of 2-4 MG.

Three graduate students perform experiments, data processing, and atomic calculations. Laboratory data for the quadratic Zeeman effect will help to benchmark the atomic spectral calculations at high magnetic fields and study strong stellar astrophysical magnetic fields.

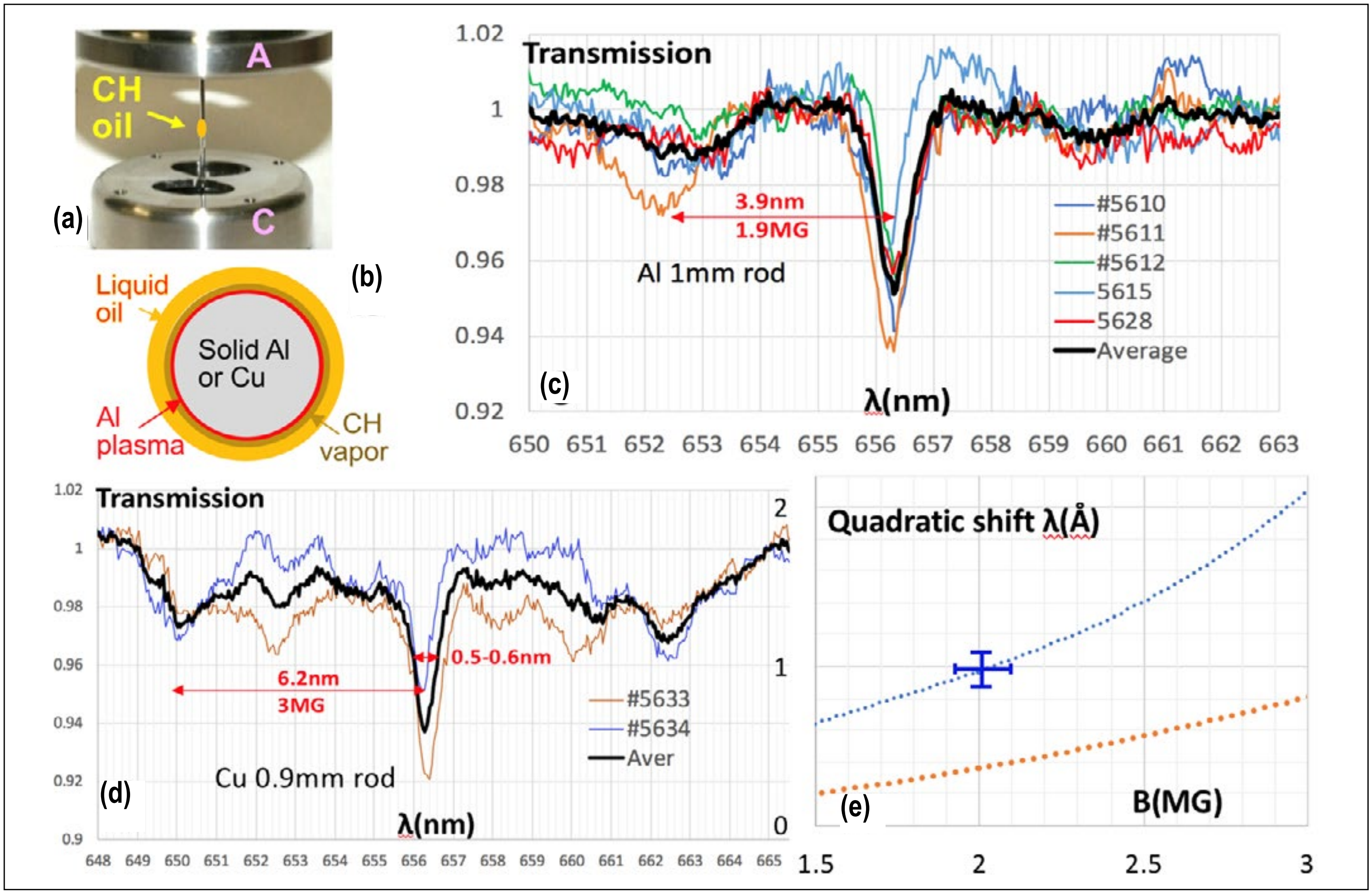


Figure 1. (a) A rod load with CH oil. (b) A cross section of the load during the shot. (c, d) An absorption H-alpha line from Al and Cu loads. (e) Calculated (lines) and measured (points) spectral shift of H-alpha (red) and H-beta (blue) lines due to the quadratic effect.

Hard and Soft X-ray Line Emission from High-Z Multiply-Ionized Ions Influenced by Dielectronic Recombination and Polarization from High Energy Density Laboratory Plasma

University of Nevada, Reno ✦ PI: Dr. A.S. Safronova (alla@physics.unr.edu), Co-PI: Dr. V.L. Kantsyrev (victor@unr.edu)

The atomic physics of high-Z, multiply-ionized ions and their application to High Energy Density Laboratory Plasmas (HEDLP) is a very important, unique, and cross-cutting subdiscipline. Better understanding of high-Z atomic physics is crucial for benchmarking modeling, designing experiments under well-controlled conditions, and developing new diagnostics. The goal of this HEDLP project is a comprehensive study of hard and soft X-ray line emission from high-Z, multiply-ionized ions influenced by such important processes as dielectronic recombination and polarization. Thanks to more than a decade of Department of Energy/National Nuclear Security Administration (DOE/NNSA) funding, the total of eighteen graduate students were supported and advanced in pulsed-power and z-pinch research including X-ray spectroscopy, imaging, and line polarization as well as modeling of atomic processes in HEDLP. Currently, three PhD graduate students are involved in this project (Figure 1). Our former PhD students are working at Los Alamos National Laboratory, Sandia National Laboratories (SNL), Naval Research Laboratory (NRL), and Mission Support and Test Services (MSTS).

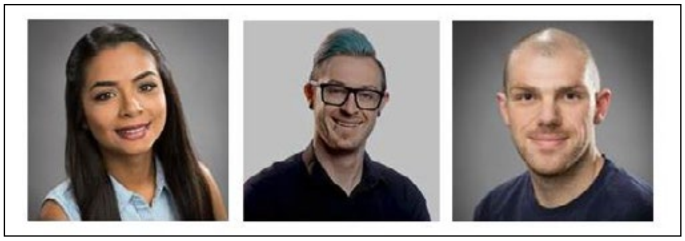


Figure 1. UNR PhD graduate students Amandeep Gill, Ryan Childers, and Chris Butcher.

Figure 2. Chris Butcher (PhD graduate student, UNR) prepares X-ray diagnostics for experiments on the laser-triggered Sparky Hard X-ray Source (HXRS) generator at UNR.

During the last few years, there was a renewed interest to study hard X-ray (HXR), non-thermal, inner-shell emission from z-pinch plasmas of high-atomic-number materials on SNL's Z and NRL's Gamble II generators. In this project, we continue such studies of fusion-important tungsten (W) using unique data on time history of relative intensities of cold L-shell lines from compact W wire arrays (produced on the University of Nevada, Reno (UNR) Zebra generator in a spectral range between 1 and 1.7 Å). It is important to gain a better understanding of non-thermal plasmas and for the development of efficient X-ray sources and new diagnostics of both "hot" HEDLP and warm dense matter.

One of the important signatures of non-thermal, high-Z plasmas is polarization of HXR line emission. Atomic processes in HEDLP and astrophysical plasmas with anisotropic electron distribution function (EDF) that can lead to such polarization include dielectronic recombination. All previous research on X-ray line polarization of dielectronic satellite (DS) lines was focused mostly on K-shell radiation. The first studies of polarization of L-shell DS lines using HXR spectra of sodium (Na)-like W were accomplished using two approaches: the Flexible Atomic Code (FAC) and the density matrix formalism[1]. Polarization-dependent DS spectra between 1.15 and 1.38 Å, calculated with a gaussian EDF centered at electron beam energies EB= 2,400-4,100 eV, were found to be strongly dependent on EB, which is essential for the development of X-ray plasma polarization spectroscopy of non-thermal W plasmas.[1]

Theoretical research of the graduate student Amandeep Gill was focused on atomic processes in highly ionized xenon (Xe) plasmas radiating between 2.5 and 14 Å. It included benchmarking of the new M-shell Xe theoretical model with two HEDLP experiments as well as a theoretical study of X-ray line polarization of L-shell Xe. In particular, polarization properties of DS spectra of Na-like Xe were studied, and the trend towards a maximum negative polarization was tested for large J-values.

During his second 5-month residency at SNL, the graduate student and Laboratory Residency Graduate Fellowship (LRGF) fellow, Ryan Childers, successfully completed a very challenging task of building a new Monte Carlo Radiation Transport Code to study non-thermal emission in high energy density (HED) plasmas. Initial simulations of cylindrically compressed Magnitized Liner Inertial Fusion (MagLIF) plasmas revealed beryllium+iron (Be+Fe) liner temperatures and Fe degree of ionization consistent with experimental diagnosis. An application of this code to different plasmas environments is in progress.

Experimental research of the graduate student, Chris Butcher, was focused in two directions: studies of W z-pinch behavior at 1 MA generators of different architecture in collaboration with the University of Michigan and SNL[2] and application of the laser-triggered Sparky HXRS generator for X-ray spectropolarimetry. His work on the development of X-ray diagnostics and spectropolarimetry on the Sparky continues (Figure 2).

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> *The HEDLP program also gave me a window into the work of the national laboratories: cutting edge science in the service of national interests. The Department of Energy/National Nuclear Security Administration (DOE/NNSA) labs leverage the biggest pulsed power accelerators, fastest supercomputers, brightest free-electron lasers, and large interdisciplinary teams with world experts in diverse fields to solve challenging and important problems.*

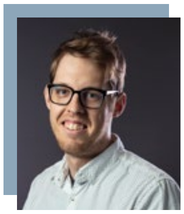
— *Dr. Trevor Hutchinson*
Lawrence Livermore National Laboratory

> *The HEDLP program is worth your time. You likely will be challenged to do more than you thought possible. While difficult, the growth in skill and expertise is exciting. The work being done is important.*

— *Travis E. Bejines*
Idaho State University

Trevor Hutchinson, Lawrence Livermore National Laboratory (hutchinson12@llnl.gov)

Years at LLNL: 2020-Present ✦ **Degree:** PhD, Physics ✦ **HEDLP:** 2019-2020, University of Nevada, Reno



I was supported by a High Energy Density Laboratory Plasmas (HEDLP) grant for two years while I was a graduate student in the plasma physics program at the University of Nevada, Reno. The grant funded me to execute experiments to understand an instability that forms in metals carrying electrical current densities greater than approximately one million amps per square millimeter. This instability, called the Electrothermal Instability (ETI)[1] generates mass density perturbations perpendicular to the electrical current that degrade magnetic direct drive approaches to inertial confinement fusion. Via HEDLP program support, I was able to identify influential initial conditions from which the ETI grows[2] and quantify how fast metals expand during electrical explosions.[3]

In my current role at Lawrence Livermore National Laboratory (LLNL), I'm working on two projects. For my first project, I am part of a team that spans LLNL and Sandia National Laboratories (SNL) and aims to improve our understanding of magnetically-assembled, inertially-confined, fusion plasmas. In this role, I'm the LLNL lead scientist for velocimetry on the Z-pulsed power facility at SNL. More specifically, I am developing techniques to infer the amount of electrical current that 'shorts' the Z electrical transmission line before it gets to a target – we believe this shorting occurs in low-density, highly-mobile plasmas that emerge from ice/metal/hydrocarbons vaporized off electrode surfaces. By building a Python wrapper around a magnetohydrodynamics code called Ares, the electrical drive conditions can be varied iteratively until computational predictions optimally match experimental data. The inferred current loss then can be used to design better experiments.

For my second project, I am part of a team supported by Laboratory Directed Research and Development (LDRD) funding that is advancing state-of-the-art, optical, velocimetry diagnostics, specifically Velocity Interferometry for Any Reflector (VISAR). The goal of this LDRD not only is to evaluate the two-dimensional (2D) velocity field of a reflecting target (as traditional 2D VISAR does) but also to recover the phase of the electromagnetic field that reflected from the target. This allows 'refocusing' of the 2D velocity image within the experimental volume, augmenting the depth of field of the diagnostic. It also permits recovery of the topography of the reflector simultaneously with the 2D velocity map. This diagnostic has the potential to quantify the non-uniformity introduced to direct drive implosions via laser speckle (laser imprint), shock-driven instabilities at corrugated interfaces (Richtmyer-Meshkov instabilities), or the influence of viscosity on the planarity of shock fronts.

> *“The HEDLP program also gave me a window into the work of the national laboratories: cutting edge science in the service of national interests. The Department of Energy/ National Nuclear Security Administration (DOE/NNSA) labs leverage the biggest pulsed power accelerators, fastest supercomputers, brightest free-electron lasers, and large interdisciplinary teams with world experts in diverse fields to solve challenging and important problems. If you love science, these are the right places, and HEDLP program is a great conduit.”*

The HEDLP program provided me the opportunity to travel to SNL to execute multi-week campaigns on the linear transformer driver, Mykonos. Additionally, I had the funding to design and build novel diagnostics, targets, and facility improvements. Finally, and importantly, the HEDLP program provided access to scientists with niche expertise who were happy to weigh-in on experimental difficulties specific to their field but tangential to mine.

The HEDLP program also gave me a window into the work of the national laboratories: cutting edge science in the service of national interests. The Department of Energy/National Nuclear Security Administration (DOE/NNSA) labs leverage the biggest pulsed power accelerators, fastest supercomputers, brightest free-electron lasers, and large interdisciplinary teams with world experts in diverse fields to solve challenging and important problems. If you love science, these are the right places, and the HEDLP program is a great conduit.

This work was performed under the auspices of the U.S. DOE/NNSA by LLNL under Contract DE-AC52-07NA27344.

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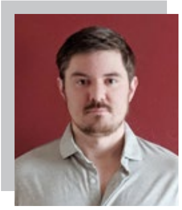
Travis E. Bejines (bejitrav@isu.edu)

Degree in Progress: PhD, Physics,Pulsed Power HEDP, Idaho State University ✦ **Advisor:** Dr. Rick Spielman ✦ **HEDLP:** 2018-Present

Research Topic

Zirconium Phase Transition Measurements on the Cinco Intermediate Pulser



Research Responsibilities

My research responsibilities are quite varied. I am responsible for many aspects of the Cinco project. My duties regularly include part design on the Computer Aided Design (CAD) platforms (currently using FreeCad), circuit calculations and design, welding and soldering, bonding and shaping acrylics, potting with epoxy, and data collection and analysis (currently using Python).

Benefits of HEDLP

The Stewardship Science Academic Programs (SSAP) is a community. While in graduate school, it is important to meet and network with others in your field of study. SSAP usually provides a great way to share your research and meet others across the country doing things related to your work.

What Students Considering HEDLP Should Know

The High Energy Density Laboratory Plasmas program is worth your time. You likely will be challenged to do more than you thought possible. While difficult, the growth in skill and expertise is exciting. The work being done is important.

New Contacts, New Opportunities

My advisors include Dr. Spielman and Dr. Reisman. Cumulatively, they have done a lot of important work, and having access to their collective knowledge and experience is incredibly valuable. Tasks that would have taken me many hours to figure out were spotted instantly by these experts, along with probable causes for what the data was telling us. They also have a lot of professional connections that can help with getting things done, especially if we need to borrow a piece of equipment to continue our work. Similarly, I have calibrated some diagnostics for others, which is an experience that I would not have gotten otherwise, and it will aid me moving forward in my career. My advisors are excellent examples of scientists and how we can work together to achieve collective goals. Most people know each other and the capabilities of their facilities.

National Laboratory Experience

The only time I spent at a national lab was for a conference at Sandia focused around the Z machine, prior to COVID-related lock-downs. As with any new experience, exposure to current work and future possibilities is beneficial. It can help guide future decisions on what research you are both interested in and what you think is important. Whereas some of the work was extremely specialized and specific, it helped me put my own research into context and to see how my machine (Cinco) compares in terms of scope and capability. It also helped me realize what types of materials would be both interesting and useful to look at when selecting materials for data collection. If you can spend time at a national laboratory, you definitely should. My reasons for not are centered solely around my family life.

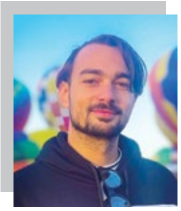
The SSAP has presented me the opportunity of expanding my research interest and forging my future career as a researcher.

Enac Gallardo-Diaz (enacgallardo@nevada.unr.edu)

Degree in Progress: PhD, Physics, University of Nevada, Reno ✦ **Advisor:** Dr. Roberto C. Mancini ✦ **HEDLP:** 2019-Present

Research Topic

Plasma Spectroscopy in Inertial Confinement Fusion Implosion Experiments



Research Responsibilities

My research consists of developing a new spectroscopic diagnostic technique that will allow us to infer hot inertial confinement fusion (ICF) implosion plasma’s electron temperatures and densities. I model high-Z elements’ (like krypton) emission spectra and study its sensitivity to these magnitudes for relevant ICF conditions. Then, at the OMEGA laser facility, we introduce tracer amounts of this element into the implosion fuel pellets and experimentally detect the emission spectra using a set of spectrometers. After analyzing this data and comparing it to the models, we can obtain a measurement of the electron temperature and density of the plasma.

Benefits of HEDLP

This program has given me the opportunity to use my research to study an approach to fusion energy that has been my dream even before starting my physics undergraduate studies. I have learned so much, and I have started to contribute to this area of research. Even in the difficult times of the pandemic, this program has allowed me to attend different conferences virtually such as the annual meeting of the American Physical Society Division of Plasma Physics. This has been important for my career through the exposure to the advances that fellow scientists are achieving in my field and knowing their opinion and feedback on my research.

New Contacts, New Opportunities

The Stewardship Science Academic Alliances (SSAA) has given me the opportunity to connect and work with a wonderful group of people from different backgrounds. We are part of a Center of Excellence focused on high energy density physics (HEDP) with members from different universities such as MIT, Virginia Tech, University of Rochester, and University of Iowa. Thanks to this center I have been able to participate in collaborations with other scientists and learn from their work as well as perform implosion experiments at the OMEGA laser. I am certain to say this has been key opportunity for my graduate training and education and my development as a scientist.

National Laser Users' Facility Grants

High Pressure and Temperature Polymorphism of a Key Super-Earth Mantle Material: MgO

Johns Hopkins University ✦ PI: Dr. June Wicks (wicks@jhu.edu)

Figure 1. The science team for this NLUF program's inaugural campaign at OMEGA-EP. Wicks' lab members supported by our collaboration from LLNL, Princeton University, and LLE.

The goal of this National Laser Users' Facility (NLUF) program is to explore the kinetic barriers to MgO phase transitions along the shock Hugoniot. FY20-21 marked our inaugural campaigns on the OMEGA-EP laser at the Laboratory for Laser Energetics (LLE), University of Rochester, where our primary objective was to carry out temperature measurements of the shock Hugoniot of MgO as a function of shock propagation direction. Bringing a large team enabled training and experimental support from other lab members from both Johns Hopkins University (JHU) and Princeton (Figure 1). This work is part of a continued collaboration between the principle investigator (PI) and scientists at Lawrence Livermore National Laboratory (LLNL) and Princeton University whose common goal is to measure crystal structure and compressibility of minerals under dynamic compression.

As one of the most important building blocks of the Earth and other rocky planets, MgO is a relevant material to characterize at extreme conditions. It serves as a high-pressure analogue for most other diatomic ionic solids for which the B1-B2 transition pressure and mechanism has been studied for decades.[1] The equation of state, phase diagram, and rheology of MgO at the extreme pressures of the B1-B2 transition (300-500 GPa) likely plays an important role in the mantle convection dynamics of Super-Earth interiors.[2]

The high pressure/temperature phase diagram of MgO has been beyond experimental reach until recent years, when groundbreaking research carried out on the OMEGA laser facility identified the B1-B2 transition using streaked optical pyrometry in decaying shock experiments[3] and then again using X-ray diffraction in laser-driven ramped compression experiments.[4] Discrepancies between experimental measurements and theoretically-predicted shock Hugoniot(s) (and implied phase diagrams) have been attributed to both kinetics and anharmonicity, exacerbated by the extreme temperatures associated with melting (~10-15 kK along the Hugoniot).[5]

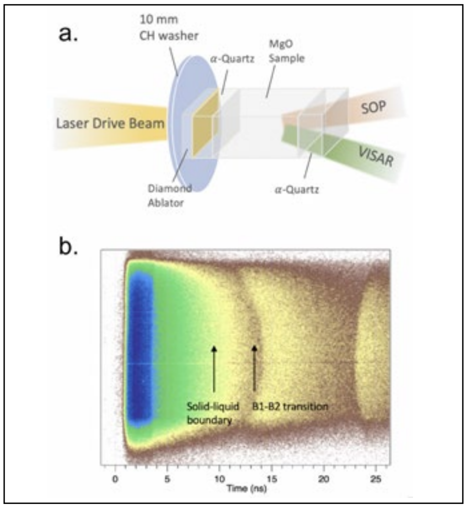


Figure 2. (a) Target setup at OMEGA-EP for decaying shock measurements of single-crystal MgO with a quartz reference material. Line VISAR measured the shock front, while (b) streaked optical pyrometry simultaneously measured the thermal emission.

In these decaying shock experiments, 1 ns laser drives are used to drive a strong but unsupported shock wave through the sample assembly (Figure 2). The propagating shock front is monitored using the line-imaging velocimetry (VISAR) and Streaked optical Pyrometry (SOP) diagnostics, where the properties of quartz windows before and after the MgO served as *in situ* calibrants[6,7] (Figure 2a). Discontinuities in the VISAR and pyrometry records delineate phase changes, enabling the identification of the B2-liquid and the B1-B2 transitions, respectively (Figure 2b).

Decaying shock measurements of MgO conducted along different crystallographic directions revealed exciting differences in the location and shape of temperature discontinuities along the shock Hugoniot, indicating different transition energy barriers as a function of orientation. Follow-up work using *in situ* X-ray diffraction will allow us to better understand the temperature trends in the second year of this program. These results will provide insight into the kinetics effects on extreme-temperature phase transitions during the timescales of shock compression. The experimental and analytical techniques developed in this project benefit stockpile stewardship science as it expands our ability to diagnose material properties at extremes of pressure and temperature, while providing new information on material states in the warm dense matter regime.

The project is of great importance for training the next-generation of scientists in high-power laser experimental techniques. A highlight of FY20 was the presentation of this project by former undergraduate researcher, Junellie Gonzalez Quiles, at the 2019 SACNAS conference, winning a best poster award. This NLUF grant provided primary support for 2nd-year graduate student, Zixuan Ye (Figure 1 inset), who spent the following summer studying under Dr. Marius Millot (LLNL) through the virtual Livermore scholars program. In this internship, she developed and applied optical absorption corrections with the eventual goal to explore transition kinetics effects on optical measurements during dynamic compression experiments.

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Characterization of Ion-Heated Warm Dense Matter and Its Ion Transport Properties

University of California, San Diego ✦ PIs: Professor Farhat Beg (fbeg@ucsd.edu) and Dr. Christopher McGuffey (christopher.mcguffey@ga.com)

This project, led by the University of California, San Diego (UC San Diego) with a co-investigator at General Atomics and unfunded contributors at the Laboratory for Laser Energetics (LLE) and Lawrence Livermore National Laboratory (LLNL), has studied the processes involving intense proton and ion beams transporting through foam or solid matter through experiments, simulations, and analytical models.

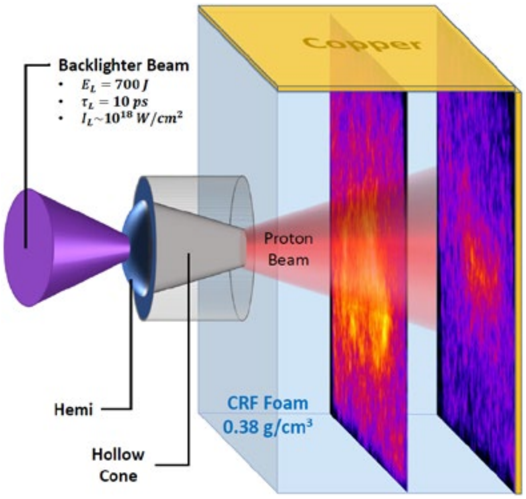

Figure 1. Depiction of the experiment to study proton transport through mm-scale foam. The OMEGA EP Backlighter laser irradiated a hemi+cone target, sending a $>10^9$ A/cm^2 proton beam into carbon-based foam. The overlays show emission images of 8 keV Cu-Kα (stretched here for visual effect) from two shots with foam length 0.55 or 1.0 mm.

Proton and ion beams can be generated efficiently by short-pulse, high-energy laser irradiation of a thin foil. When sufficiently intense, the particle beam can heat a material sample rapidly into a partially- or fully-ionized, dense state. Behavior of the beam in this scenario is difficult to predict due to the uncertain properties of warm, dense matter (WDM). Proton-heated samples could be used as in-laboratory WDM surrogates for inertial confinement fuel and planetary cores.

LLE's OMEGA EP Backlighter is one of the lasers utilized in this project, because its parameters are suitable for producing proton beams with > 20 J beam energy, enough to heat samples of mg-scale mass to >1 eV. By incorporating a hollow cone into the target design ("hemi+cone"), the beam can be focused and can heat samples locally to >100 eV.[1]

In another OMEGA EP experiment, hemi+cone targets were used to focus protons into plastic foam samples to investigate their propagation through matter. As shown in Figure 1, the hemi+cone was attached to the front of the foam which was either 0.55 or 1.0 mm in length. Cu foils were attached on the top and rear of the foam, and their Cu-Kα emission was imaged. A spot was seen, indicative of an intact beam of protons and/or electrons. Changes between the profiles at the two depths can be used to discern transport of the beam.

Graduate student, Krish Bhutwala, led a simulation study of the beam/foam interaction. To simulate proton transport and heating, a proton source was synthesized with energy spectrum closely matching the measured spectrum from a hemi+cone target without a sample. Instead of applying a simple source angle for the beam, several energy bins were assigned individual differential angular spectra. Electron simulations also were conducted, and synthetic Cu-Kα maps were generated through additional simulation and post-processing. Results showed that the accelerated protons dominate over the electrons in heating the foam significantly, and they also are responsible for much of the Cu-Kα peak observed in the experiment.[2]

In the third year of the project, experiments were conducted at OMEGA EP to measure the instantaneous opacity of proton-heated Si[3] and at the Vega II 200 TW laser to measure proton stopping power in warm, dense carbon. A previously published work[4] on heating with the protons from a short pulse laser was featured as an Editor's pick in the *Transactions of Plasma Science* Email Blast.

Mr. Bhutwala and Dr. Joohwan Kim also are developing an analytical framework intending to model a variety of particle beam/matter transport scenarios including heating, field generation, and beam focusing. Such a tool will be useful in predicting collective effects of proton beam transport in ultrahigh current density applications such as fast ignition inertial confinement fusion.

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> *“I am excited to work on commissioning experiments, to engage with external users, and to help mentor undergraduate and graduate students involved in research activities. Along my academic journey, the support of the NLUF program has been an essential part of my development as a scientist, and I am grateful for the invaluable training and opportunities.”*

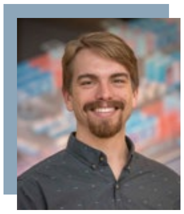
— *Dr. Paul T. Campbell*
ZEUS Laser Facility

> *“Through the NLUF program, my advisor gave me the opportunity to work with scientists at national laboratories, and she made great efforts to make the resources accessible to me, such as visiting Lawrence Livermore National Laboratory (LLNL) and conducting experiments at the OMEGA EP laser facility at the University of Rochester.”*

— *Zixuan Ye*
Johns Hopkins University

Paul T. Campbell, ZEUS Laser Facility, Center for Ultrafast Optical Science, University of Michigan (campbpt@umich.edu)

Years at Facility: 2021-Present ✦ **Degree:** PhD, Applied Physics ✦ **NLUF Program:** 2016-2019, University of Michigan



As a graduate student at the University of Michigan, I had the good fortune to work on a project supported by the National Laser Users' Facility (NLUF) program. We were granted the opportunity to use the OMEGA EP laser facility at the Laboratory for Laser Energetics (LLE) to study the dynamics of magnetic fields generated during high power laser-plasma interactions. Before starting graduate school, I never anticipated having the chance to participate in experiments at one of the world's biggest laser facilities. Though initially daunting, the training I received gave me the confidence to help lead these large-scale experiments from the brainstorming sessions and design phases through to execution on shot days. Plus, the NLUF program promotes engagement with experts at the Department of Energy/National Nuclear Security Administration (DOE/NNSA)-supported laboratories. For example, we conducted experiments at OMEGA EP to study magnetic fields generated in plasma conditions relevant to inertial confinement fusion (ICF). Using proton deflectometry measurements, we observed unique field generation dynamics as we varied the target composition. Working closely with scientists at LLE and Lawrence Livermore National Laboratory, as well as an international team, we found that radiation effects led to magnetic field generation around double ablation fronts in mid-Z materials (P. T. Campbell et al., *Physical Review Letters* 125, 145001 (2020)). These exciting experiments showed that measurements of magnetic field dynamics can help diagnose the interplay of radiation effects and heat flow in ICF-relevant plasmas and fostered continuing collaborations with scientists at the DOE/NNSA laboratories.

> *“In addition to gaining access to world-class facilities, I was afforded the opportunity to present my results at numerous conferences, including the American Physical Society Division of Plasma Physics meetings and the International Conference on High Energy Density Laboratory Astrophysics in Japan.”*

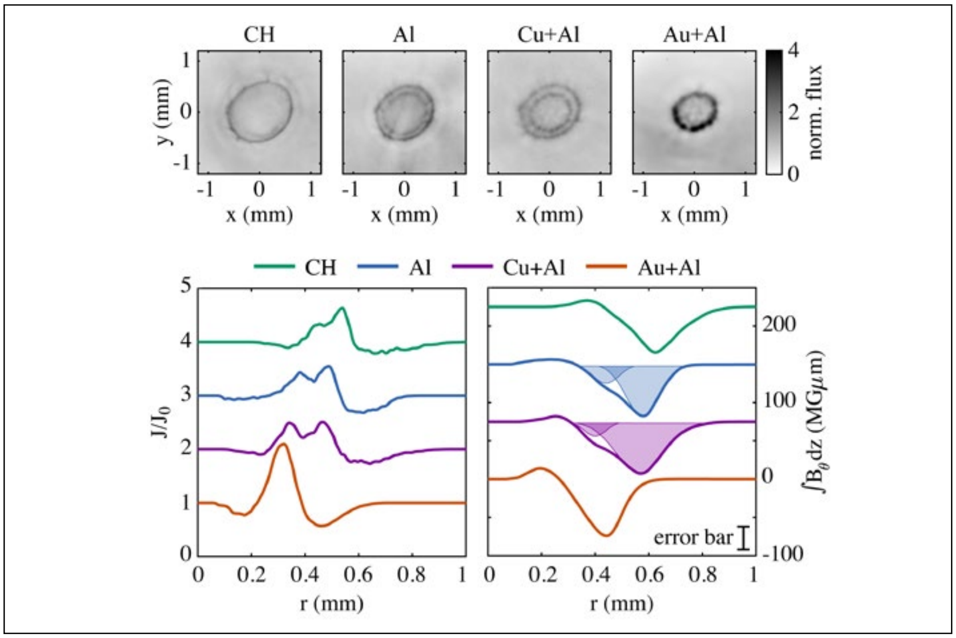


Figure 1. Proton images (top row) and magnetic field reconstruction analysis (bottom row) are compared for the different target materials at t_0 + 0.75 ns. Path-integrated magnetic field profiles (bottom right) are reconstructed using radial line-outs from the proton images (bottom left). Magnetic field generation around double ablation fronts was detected with Al and Cu+Al targets. Reprinted from P.T. Campbell et al., *Physical Review Letters* 125, 145001 (2020).

The NLUF program empowers students to make important contributions to the high energy density (HED) and plasma physics communities. In addition to gaining access to world-class facilities, I was afforded the opportunity to present my results at numerous conferences, including the American Physical Society Division of Plasma Physics meetings and the International Conference on High Energy Density Laboratory Astrophysics in Japan. After graduating, I continued studying high power laser-plasma interactions and charged-particle deflectometry as part of the DOE Fusion Energy Sciences Postdoctoral Research program. Now, I've joined the team of scientists working to build the Zettawatt-Equivalent Ultrashort Pulse (ZEUS) laser system. At peak power of 3 Petawatts, the ZEUS laser will be the most powerful in the US and among the most powerful lasers in the world. The name ZEUS refers to the collision of a Petawatt laser pulse with a beam of GeV-energy electrons that can be accelerated by one of its two beamlines. This geometry will result in the equivalent of a “Zettawatt” power laser interaction (10^{21} Watts) in the rest frame of the relativistic electron beam. ZEUS will operate as a user facility sponsored by the National Science Foundation, and the laser system will enable experiments exploring ultrafast material dynamics, acceleration of energetic ion beams, and relativistic laboratory astrophysics. I am excited to work on commissioning experiments, to engage with external users, and to help mentor undergraduate and graduate students involved in research activities. Along my academic journey, the support of the NLUF program has been an essential part of my development as a scientist, and I am grateful for the invaluable training and opportunities.

Zixuan Ye (yzixuan1@jhu.edu)

Degree in Progress: PhD, Mineral Physics, Johns Hopkins University ✦ **Advisor**: Dr. June Wicks ✦ **NLUF**: 2018-Present

Research Topic

High-pressure Properties of Minerals under Dynamic Compression

Research Responsibilities

In my role as a graduate research assistant, I conduct research on materials' properties under extreme pressure and temperature conditions using laser-driven shock compression techniques. I design experiments with the help of hydrocode simulation, prepare the sample PXRDIP (Powdery X-ray Diffraction Image Plates) boxes, and perform experiments at Omega EP, Laboratory for Laser Energetics (LLE) at Rochester University. As a shot day PI, I communicate with the technicians and shot director at LLE.

Benefits of NLUF

As a part of the National Laser Users' Facility (NLUF) program, I was given the chance to work on a great project and to do research on leading-edge science that I wouldn’t have been able to do otherwise.

What Students Considering NLUF Should Know

Before I went to graduate school, I was applying for a PhD program on mineral physics with static compression techniques (e.g., Diamond Anvil Cell). I began to be interested in dynamic compression after reading my advisor’s published papers. The leading-edge science my advisor’s been doing greatly motivated me to choose to study shock physics.

Figure 1. Zixuan Ye building a PXRDIP box for a MgO shock compression experiment for her PhD thesis at Omega EP, Laboratory for Laser Energetics at Rochester University.

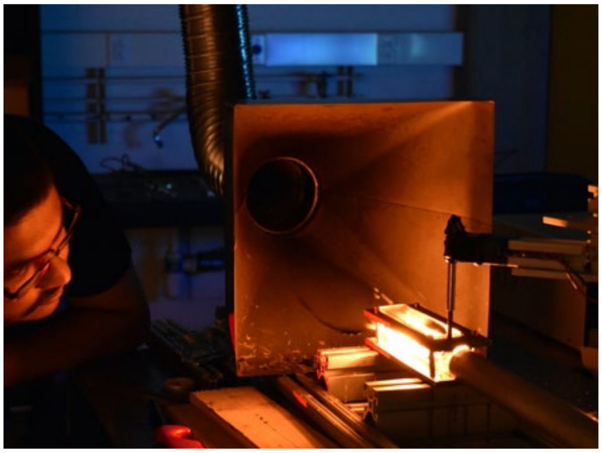
New Contacts, New Opportunities

Through the NLUF program, my advisor gave me the opportunity to work with scientists at national laboratories, and she made great efforts to make the resources accessible to me, such as visiting Lawrence Livermore National Laboratory (LLNL) and conducting experiments at the OMEGA EP laser facility at the University of Rochester.

National Laboratory Experience

I spent a summer (July-September 2020) as an intern at LLNL under the mentorship of Dr. Marius Millot. Due to the Covid policy, the internship program was about to be canceled, but, in the end, was hosted remotely. My mentor organized daily meeting with me at which he gave me guidance on the research project. I reported my research updates to him and received feedback from him. Thanks to this internship, we have made great progress on our project. During my internship, Marius gave me advice on designing experiments for our shot day in October 2020. This internship provided me with the chance to collaborate with experts from LLNL. We have continued collaborating on multiple projects after the internship ended.

Predictive Science Academic Alliance Program III



CESMIX: Center for Exascale Simulation of Material Interfaces in Extreme Environments

Massachusetts Institute of Technology ✦ PI: Dr. Youssef Marzouk (todd.palmer@oregonstate.edu)

The Center for Exascale Simulation of Materials in Extreme Environments (CESMIX) is a single-discipline PSAAP-III center 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 the degradation of complex materials in extreme environments, from first principles. 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. This setting is generally inaccessible to direct experimental observation. Significant research has been devoted to the development of better protective materials for hypersonic flight. Diborides such as HfB2 and ZrB2 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. CESMIX is addressing these challenges by developing a comprehensive new *multiscale materials simulation framework*, bridging from multiple levels of electronic structure theory to hybrid quantum/classical methods to classical molecular dynamics.

A key effort over the past year has been the design/development of an *integrated molecular simulation workflow* that emphasizes ease of use, performance, and the ability to add new technologies while making use of existing software. This framework is written in Julia, a high-level programming language, but emphasizes interfaces and abstractions that will allow for inter-operability and composability of multiple density functional theory codes (e.g., QuantumESPRESSO, TeraChem, and the Julia-native DFTK.jl), molecular dynamics simulators (LAMMPS and our in-house code MDP, as well as Julia-native simulators), and a variety of different interatomic potentials (ranging from ACE and SNAP to graph neural network potentials). Another emphasis of this framework is uncertainty quantification, at multiple scales. Our team is developing probabilistic methods for assessing model error in DFT predictions, Bayesian methods for learning interatomic potentials, and forward uncertainty propagation methods for molecular dynamics-predicted observables.

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).

Another key CESMIX effort has involved the pervasive use of *differentiable programming*. To this end, we have been expanding the scope and capabilities of Enzyme, an automatic differentiation compiler plugin for the LLVM compiler framework capable of synthesizing gradients of statically analyzable programs expressed in the LLVM intermediate representation (IR). Enzyme differs from other automatic differentiation pipelines in that it operates at a lower level—directly on an optimized, language-independent representation of code. This approach yields substantial performance increases and broader (language-independent) applicability. We have been using Enzyme within our C++ and Julia codes, and are applying it to legacy codes in our software stack as well. Other PSAAP-III centers have also begun using Enzyme.

Many additional research efforts are underway in CESMIX as we build towards our first round of system-level predictions. CESMIX researchers are *benchmarking DFT functionals* for Hf, B, and their oxides, and comparing them against higher levels of theory. We have also embarked on an experimental campaign to obtain much-needed *validation data* for high-temperature Hf oxidation kinetics, via thermogravimetric analysis. In parallel, we have been advancing our *hypersonic flow simulation* capabilities, which are aimed at generating realistic loading conditions for our materials. To this end, our first simulation target has been 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 surface heating. Having run this test case with equilibrium state models, we have begun expanding our hypersonic flow simulation code (Exasim) by coupling it with a library that provides thermodynamic, transport, and chemical properties of nonequilibrium flow and reacting surfaces.

CESMIX participants include eight faculty co-PIs, spanning five MIT departments (Aeronautics and Astronautics, Chemical Engineering, Computer Science, Mathematics, and Mechanical Engineering) and two centers (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. The rest of the CESMIX team comprises four research scientists (including a chief software architect), four postdoctoral associates, roughly eight graduate students, and even some part-time undergraduate researchers, along with several external collaborators.

Center for Exascale Monte Carlo Neutron Transport

Oregon State University ✦ PI: Dr. Todd Palmer (todd.palmer@oregonstate.edu); Author: Dr. Ryan G. McClarren, Deputy Director of CEMeNT (mcclarr@nd.edu)

Predicting the behavior of neutrons has been of fundamental importance for the nuclear security enterprise since the very beginning. Though we have come a long way from the days of using a series of wheels to simulate the movement in neutrons in a system, as Fermi did, Monte Carlo simulations that use random numbers to estimate the behavior of neutrons in a nuclear system still are a critical technology in the nuclear analytical toolkit.

Despite the inordinate progress made in Monte Carlo methods for neutron transport problems since the days of the Manhattan Project, there still is a host of open research questions. Paramount among these is how these methods scale with the next-generation of supercomputers based on hardware that often penalizes non-deterministic programs. That is, can Monte Carlo still be a useful technology if exascale performance only can be achieved for non-random algorithms?

Taking up this charge with a specific focus on neutron transport for dynamic problems where the time-dependence of neutron interactions is key is the Center for Exascale Monte Carlo Neutron Transport (CEMeNT). This Focused Investigatory Center (FIC) in the Predictive Science Academic Alliance Program (PSAAP) of the Department of Energy/National Nuclear Security Administration (DOE/NNSA) is a coast-to-coast collaboration between Oregon State University, the University of Notre Dame, and North Carolina State University. Upon viewing their list of research goals, it is clear that the team does not lack ambition, as this center aims to leverage computer science and machine learning technologies, advances in Monte Carlo transport for static problems, novel hybrid Monte Carlo-deterministic methods, and state-of-the-art verification, validation, and uncertainty quantification (VVUQ) to attack the problem. The team consists of computational scientists, applied mathematicians, and computer scientists due to the inherently multidisciplinary nature of the neutron transport problem. A key goal of the center is to train the next-generation of thought leaders in the DOE/NNSA mission space.

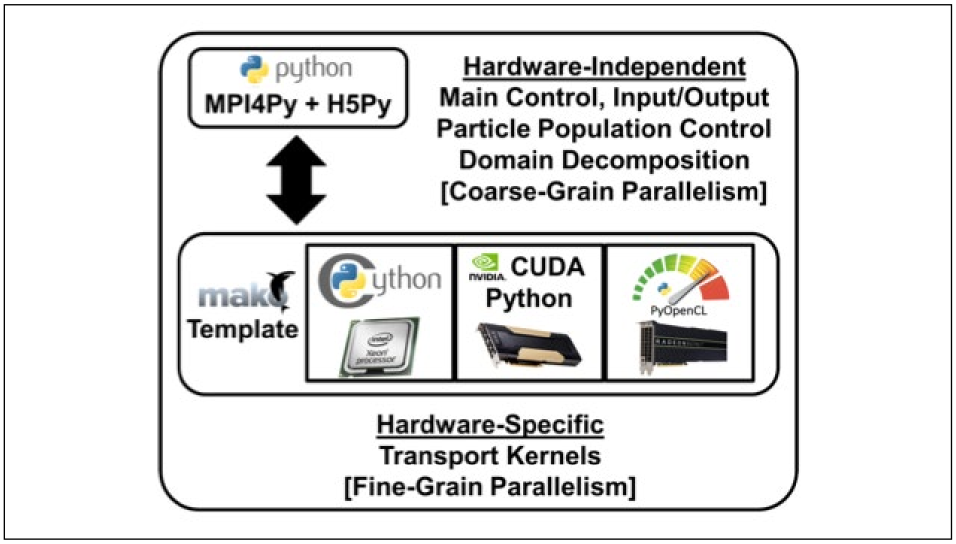


Figure 1. Diagram of the metaprogramming techniques being explored for Monte Carlo neutron transport problems at CEMeNT.

The center has notched several key successes in its first year of operation. In terms of computational methods, the team has demonstrated that using quasi-random sequences in Monte Carlo simulations can demonstrate faster convergence than the previously ineluctable slow convergence of the variance in Monte Carlo simulations, pioneered new techniques that combine the successes of previous DOE/NNSA investments in deterministic neutron transport and Monte Carlo, and provided new rigor and insight into the problem of controlling the computer memory used in a simulation with neutron population control techniques.

The successes are not limited to algorithmic improvements. The team has made progress in adapting wins from the nuclear energy side of DOE by building on the SHIFT code out of Oak Ridge National Laboratory for static neutron problems to demonstrate the challenges and opportunities unique to dynamic neutron transport. In parallel, so to speak, the center has demonstrated that novel metaprogramming techniques, as detailed in Figure 1, can be used to take Python-based codes and generate performant code on different architectures. All of this work is progressing hand-in-hand with the computer science thrust area of the center, which is taking dynamic scheduling and machine-learning-based approaches to resource allocation.

Finally, the center is aware that their research needs to be rooted in VVUQ for there to be a wider impact on the DOE/NNSA complex. In this area the team is working to demonstrate their techniques on experiments of neutron-irradiation of targets known as the pulsed sphere experiments. Moreover, they have developed a tight collaboration with Sandia National Laboratories (SNL) to implement novel, embedded uncertainty estimation techniques in the center's codes as a way to battle-test the ideas before investing in implementing the ideas in SNL's extant codes.

The next year promises further progress for the center. If this past year is any indication, we can be confident that with CEMeNT progress in important Monte Carlo simulations relevant to the DOE/NNSA mission is on solid footing.

Integrated Simulations Using Exascale Multiphysics Ensembles

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

The objective of the Predictive Science Academic Alliance Program (PSAAP)-III Center at Stanford University, Integrated Simulations using Exascale Multiphysics Ensembles (INSIEME), is to exploit Exascale computing systems to predict a complex, multiphysics phenomenon with combined innovations in task-based programming, runtime environments, physical models, numerical algorithms, data analysis, learning-at-scale and uncertainty quantification. The Center is comprised of faculty and researchers from Stanford, University of Colorado Boulder, and Purdue University.

The overarching problem of the INSIEME PSAAP-III Center is the prediction of reliability of ignition of a methalox rocket engine at high altitudes (Figure 1). Successful and repeatable ignition is key to attitude control and injection of spacecrafts in orbit.

We focus on a revolutionary ignition method that employs miniaturized, nano-second, high-energy laser pulses. This is a promising technology currently under active development in the space industry, but the existing reliability assessments have been based mostly on physical prototyping. The Center's goal is to enable simulation-based predictions of laser-induced ignition reliability by using high-fidelity physics solvers that can operate in exascale computing environments and be ported seamlessly across heterogeneous supercomputers. The Center's simulation strategy is based on the construction of a large ensemble of simulations with different levels of physical fidelity. Task-based programming is 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 — to achieve more seamless performance from next-generation supercomputers. By taking advantage of task concurrency, hardware mapping, and statistical correlations, the technical breakthrough we are pursuing is to combine all these multi-fidelity simulations to predict the reliability of laser-induced ignition using a single ensemble run.

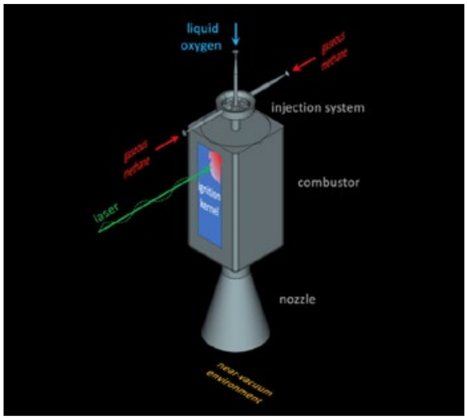


Figure 1. Computer-aided design schematics of the INSIEME experimental rocket-combustor geometry (courtesy of Carson Slabaugh, Purdue University).

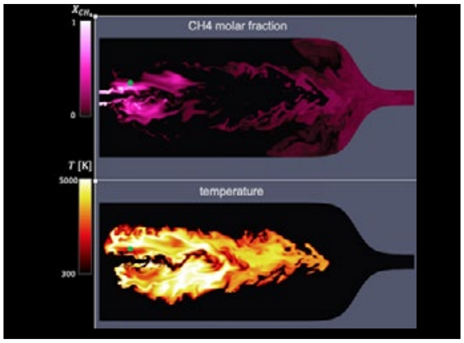


Figure 2. 3D simulations of a INSIEME PSAAP-III rocket combustor prototype run with HTR on 128 GPUs with 90% efficiency at LLNL's Lassen Supercomputer showing a successful ignition sequence. The location of laser-energy deposition is depicted by the green dot in both panels.

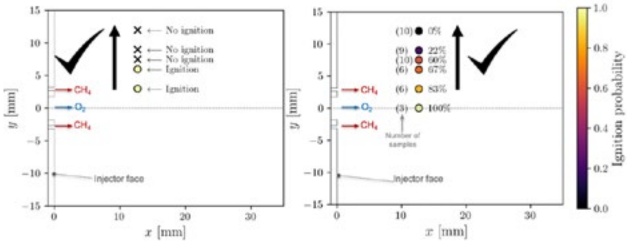


Figure 3. Simulation (left, single shot per location) and experiments (right, multiple shots per location) ignition maps in a prototype of the INSIEME PSAAP-III rocket combustor.

Our objective is to produce verified and validated ignition probability maps in the combustor, which are obtained from approximately 100,000-1,000,000 concurrent multi-fidelity computations on exascale machines with an efficient, portable, high performance computing (HPC) code. The ensembles employ a heterogeneous set of simulations (including Direct Numerical Simulations (DNS), Large Eddy Simulations (LES), Reynolds-Averaged Navier Stokes (RANS), coarse simulations, and reduced-order models) and are constructed by accounting for intrinsic uncertainties in the system, including variabilities in laser energy, focal position, deposition time/interval, propellant inflow conditions, chamber pressure, geometry, etc. To achieve this goal, the INSIEME PSAAP-III Center currently is undertaking research activities in several technical disciplines, including Computer Science, Flow Physics, Uncertainty Quantification, Data Science, and Verification & Validation.

In the first year of operation of the INSIEME PSAAP-III Center, 1) we stood-up full-system simulations on multiple graphics processing units (GPUs) with 90% efficiency using our in-house task-based Hypersonic Task-based Research (HTR) code for compressible, chemically-reacting flows (Figure 2), 2) we introduced and verified enhanced numerics/physics capabilities in HTR, 3) we designed combustor prototypes and completed O(100) experimental tests, 4) we carried out initial comparisons to experimental pressure signals and ignition probability maps in the combustor (see Figure 3), 5) we designed and implemented a Legion-based automapper for improved performance on heterogeneous supercomputers, 6) we deployed a continuous integration/continuous delivery (CI/CD) methodology in our software development process to enhance portability on multiple DOE/Stanford systems, 7) we demonstrated a prototype of Legion-based multifidelity ensemble co-processing on heterogenous systems, 8) we designed Legion-based multiblock grid capabilities, 9) we introduced an interactive browsing tool for ensemble data analysis, and 10) we initiated embedded machine-learning-based modeling for spray atomization with positive results.

Year one has been a fruitful period of collaborations between the INSIEME PSAAP-III Center and DOE/NNSA laboratories thanks to the internship program. Earlier in Summer, one of our top graduate students in the Center participated in an internship at Los Alamos National Laboratory's XCP Division where he developed novel, large-scale simulations of transitional, triple-point shock interactions using our in-house HTR code. We look forward to a year two of the PSAAP-III Program sure to be full of exciting research and developments.

Center for Hybrid Rocket Exascale Simulation Technology

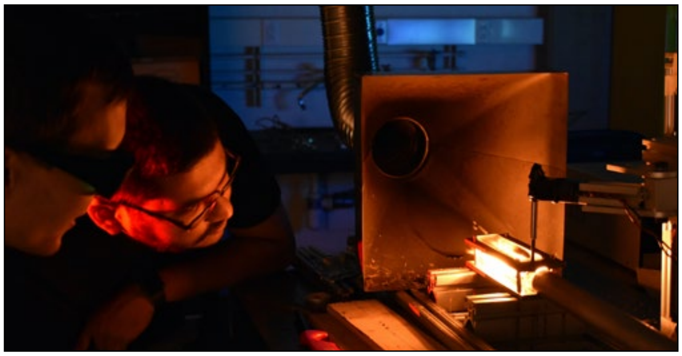
University of Buffalo ✦ PI: Dr. Paul DesJardin (ped3@buffalo.edu)

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 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. The single discipline center, the Center for Hybrid Rocket Exascale Simulation Technology (CHREST) was formed to explore the turbulent reacting flow physics of hybrid rocket motors using exascale computing and employing model reduction strategies based on machine learning for design optimization and uncertainty quantification.

CHREST brings 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 rocket motors to enable a next-generation of low-cost space flight. One promising option is hybrid rocket motors that can provide a sought-after blend of 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. The focus of the center for the first couple of years is to study these processes and to simulate them from first principles.

Year one efforts of the center have been focused on both experimental and numerical analysis of a well-characterized, small-scale slab burner. The slab burner consists of a gaseous, oxygen-fed combustion chamber and a solid paraffin wax fuel shown in Figure 1a. The appeal of the burner is full optical access to the regressing fuel interface allowing for detailed field measurements of fuel regression rates using machine-learning-based algorithms. Figure 1b shows results from two-color pyrometry for simultaneous measurements of temperature and velocity, coupled with ray tracing algorithms for experimental determination of heat transfer to the fuel surface.

The insights from the slab burner experimental work, along with uncertainty analysis of measurements, has driven the development of the CHREST's collaborative software framework, Ablative Boundary Layers At The Exascale (ABLATE). ABLATE is based on modern software principles and is designed to enable exascale simulations on modern architectures. ABLATE has been exercised on a variety of machines at UB and at the Department of Energy/National Nuclear Security Administration (DOE/NNSA) national laboratories. ABLATE components consist of low- and high-Mach computational fluid dynamics (CFD) solvers, prediction assessment modules, and several subgrid scale models to account for shear-driven atomization and combustion phenomena. Figure 1c presents preliminary results showing flame dynamics over the paraffin wax fuel slab using a reduced chemical kinetic mechanism. Current efforts are focused on expanding these simulations with: 1) more complex chemistry, 2) fuel atomization dynamics, and 3) uncertainty quantification of measurements and models. The chemistry is being expanded using customized kinetic mechanisms via model surrogates and adaptive tabulation techniques using neural networks. Fuel atomization is being modeled by combining volume of fluid descriptions of wave instability dynamics with semi-analytical models of droplet pinch-off. The combination of these efforts will lead to an integrated simulation tool to study, in detail, the critically important fuel atomization and combustion phenomena of high regressing fuels in hybrid rocket motors. More details can be found at: https://buffalo.edu/chrest.



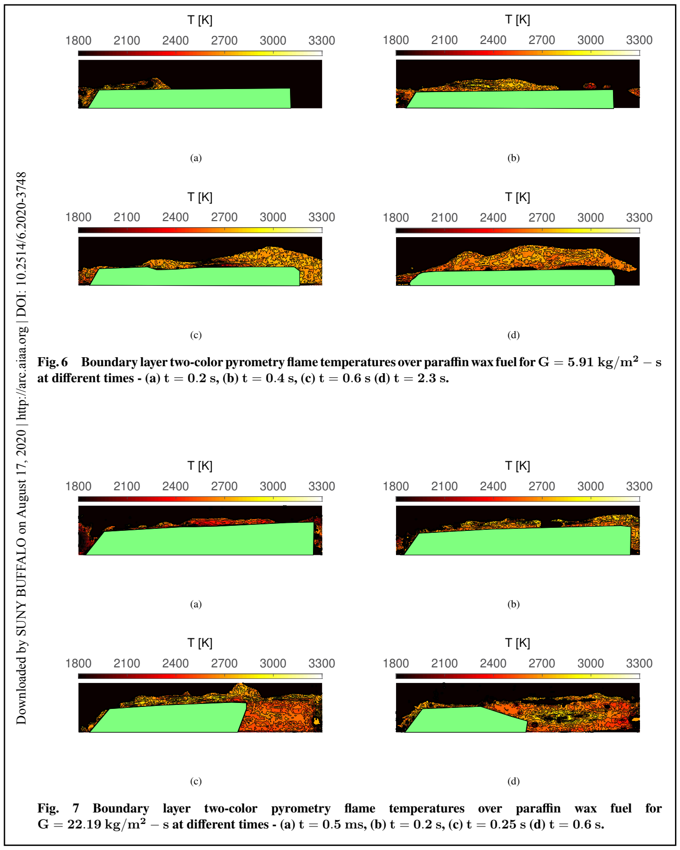


Fig. 6 Boundary layer two-color pyrometry flame temperatures over paraffin wax fuel for $G = 5.91\ \mathrm{kg/m^2 - s}$ at different times - (a) t = 0.2 s, (b) t = 0.4 s, (c) t = 0.6 s (d) t = 2.3 s.

Fig. 7 Boundary layer two-color pyrometry flame temperatures over paraffin wax fuel for $G = 22.19\ \mathrm{kg/m^2 - s}$ at different times - (a) t = 0.5 ms, (b) t = 0.2 s, (c) t = 0.25 s (d) t = 0.6 s.

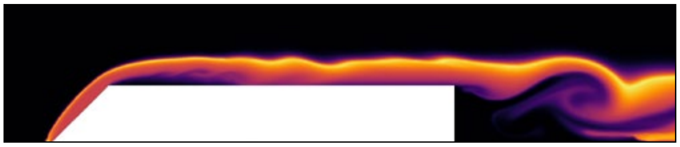


Figure 1. CHREST milestone 1 efforts showing (a) slab burner experiment, b) two-color pyrometry measurements, and c) predictions using newly developed ABLATE framework.

Center for 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 Multidisciplinary 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 and fragmentation of unbonded and bonded particulate materials. The overarching problem is to quantify processing effects on thermo-mechanical behavior of compressed pristine and recycled mock high explosive (HE) material subjected to quasi-static and high-strain-rate confined and unconfined compression, in-situ and ex-situ laboratory and synchrotron X-ray imaging and computed tomography (CT), and dynamic Kolsky bar experiments with ultrafast and high-speed imaging at the Advanced Photon Source (APS), Argonne National Laboratory (ANL). The mock HE is composed of a mixture of ~1 mm diameter agglomerated prills of idoxuridine (IDOX, average particle diameter ~200 micrometers) mixed with polymeric estane binder.

To accomplish the objective, a micromorphic, multiphysics, multiscale computational framework is being developed, verified, and validated with quantified uncertainty and executed on exascale computing platforms through a scientific software workflow to reduce the effort on handling data from the beginning to the end of simulation. Machine Learning (ML) algorithms will be applied to fill 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) 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, heterogeneous central processing unit-graphics processing unit (CPU-GPU) computing is needed to simulate these more sophisticated micromorphic, multiphysics, bridged-DNS simulations, with offline machine learning (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.

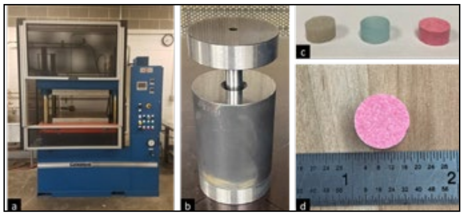


Figure 1. (a) Genesis hydraulic press; (b) half inch die; (c) from left to right: F50 sand in FK-800 resin, plain epoxy, and recycled IDOX mock HE; (d) recycled IDOX mock HE with ruler for scale.

Some highlights from Year 1 include: (i) fabricating a 0.5 inch die press at the Colorado School of Mines to mimic thermal pressing of mock HE at Los Alamos National Laboratory (LANL) (Figure 1) with associated quasi-static and dynamic unconfined compression experiments for model calibration (Clarke, Camerlo, Becker, Wallace); (ii) development and initial testing on F50 sand of a single particle, quasi-static compression apparatus at the University of Tennessee Knoxville to fit within the beamline at the APS for *in-situ* CT (Alshibli, Hicks); (iii) development and initial testing on glass beads in epoxy of a stopper fixture for interrupted high-strain rate Split Hopkinson Pressure Bar (SHPB) experiments at the University of Texas Dallas (UT Dallas) (Lu et al.); (iv) implementation of additional hyperelastic constitutive models into libCEED+PETSc for CPU-GPU computing (Brown, Thompson, Stengel at University of Colorado Boulder (CU Boulder); thermo-visco-elasto-plastic-damage models to be implemented later); (v) performance testing and usage of GEOS-MPM for simulating particle compression (glass beads, and F50 sand to start) with associated voxel-to-MPM-point map for easier discretization of CT data (Figure 2, Appleton, Tufo, Regueiro at CU Boulder); (vi) development of multiscale micromorphic continuum finite element method (FEM) code Tardigrade (Miller, LANL and CU Boulder, Regueiro); (vii) creating post-processing tools to analyze network statistics varying spatially and temporally during LAMMPS DEM simulations (Figure 3) for evolution of fabric to inform the statistically-based branch of a micromorphic model in Tardigrade (Lamont, Vernerey, CU Boulder); (viii) developing an approach for fracture detection within micromorphic Tardigrade code (Schaefferkoetter, Song, CU Boulder); (ix) implementation of Embedded Finite Element Method (EFEM) into MOOSE (Arunachala, Linder, Stanford); (x) developing and verifying a generative modeling-based method (GenMod) for polynomial chaos (PC) expansion in the presence of high-dimensional random inputs (Wentz, Doostan, CU Boulder); and (xi) generating scanning laser vibrometry calibration and test data for data-driven modeling and beginning the implementation of Physics-Informed Neural Networks (PINNs) to estimate QoIs from laser ultrasonics data (Schmid, Pourahmadian, CU Boulder).

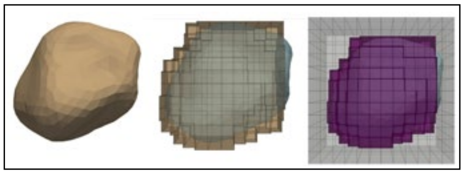


Figure 2. Left to right: PyVista workflow for voxelization of CT data to MPM points.

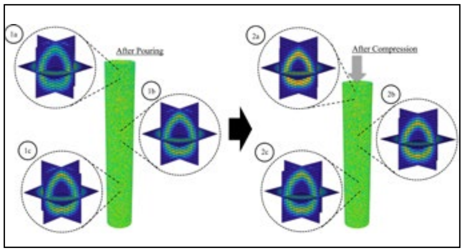


Figure 3. Branch vector distribution at representative heights before and after compression (LAMMPS DEM). Densification is clearly observed in the top part of the cylinder, while the bottom part remains unchanged.

Some MSC activities for FY 2022 include: (1) improving integration of experiments, modeling, and UQ efforts across the Center; (2) moving experimental efforts to focus on F50 sand and Estane binder and mock HE (idoxuridine (IDOX) crystals and Estane binder) with associated modeling; (3) streamlining the transition of grain-scale CT geometry identification from raw voxelized data to numerical discretization such as MPM points; (4) implementation of implicit MPM into libCEED; (5) planning for GPU extension of ParaEllip3d-CFD, with particle fracture, and possibly level set particle shapes; (6) discretization of binder into grain-resolved GEOS-MPM and LAMMPS DEM models; (7) examining and introducing equivariance convolutional neural network and transformer to ensure material frame indifference and material symmetries for deep learning predictions, and deploying trained neural networks to DNS codes libCEED, GEOS-MPM/GEOSX, LAMMPS DEM, and ParaEllip3d-CFD.

Center for Exascale-enabled Scramjet Design

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

Scramjets are an enabling propulsion technology for hypersonic flight and access to space. As for any flight vehicle, weight efficiency is critical for performance which motivates the center's planned, multi-physics, predictive simulation to evaluate the use of lightweight, high-temperature, carbon-fiber composites in scramjet combustors.

Predictive confidence through the resolution of physics length and time scales depends on efficient use of available computational resources. To do this, the center is developing a novel computer science approach, which seeks to preserve flexibility in the face of increasingly complex computational hardware. The governing equations are expressed in Python drivers that represent the computational kernels of the discretization. These are flexible in their expression and adhere to straightforward rules. The driver and kernels layers are human readable, directly crafted by the computational scientist and those implementing the details of the numerical discretization, as they would have been in most historical applications. The computational kernels then are processed automatically into a polyhedral loop abstraction, which, in turn, allows them to be systematically analyzed to establish lazy evaluation patterns that facilitate efficient mapping to available hardware. For current accelerator-based architectures (e.g., Lawrence Livermore National Laboratory's (LLNL) Lassen), this means fusions into large kernels that minimize data movement. Code is then generated (currently in OpenCL) to run on available devices. This approach is called MIRGE for Math—Intermediate Representation—Generation—Execution.

In its first year, the center has developed within this framework MIRGE-Com, a new Discontinuous Galerkin flow and combustion solver, and an initial lazy evaluation traversal of it has been demonstrated to generate code that runs on Lassen graphics processing units (GPUs). Another Illinois tool, Pyrometheus, generates lightweight code for specific combustion chemistry based on the extensive Cantera combustion kinetics package. A meshing and simulation workflow has been established, and the workflow management tool, Parsl, is being evaluated for orchestrating multi-stage simulation and uncertainty quantification workflows, with the option of doing this via Jupyter notebooks. New non-expert users successfully have implemented methods for shock capturing and alternate governing equations (heat equation), demonstrating the accessibility of the computational scientists' facing side of the framework. Daily verification tests cover nearly all code as it is developed and track performance histories for simulations representative of anticipated annual predictions.

In parallel with the simulation development, physical models are being integrated for the oxidation surface kinetics of carbon fibers, fracture dynamics of the degrading wall material, and thermal transport into the composite wall materials. These models are tightly linked with physics-targeted experiments for calibration and validation (Figure 1). An initial combustion chemical kinetics model has been selected, and it is being evaluated critically for its uncertainty in the application predictions. An end-to-end uncertainty quantification workflow has been established, which leverages the low-dimensional, physics-targeted configurations for reduction of the uncertainty space through sensitivity analysis. Experimental data from in the Arc-heated Combustion Test rig II (ACT-II) supersonic combustion facility on the Illinois campus is acquired to provide the center's next annual prediction target.

Overall, there are 19 PhD students working within the broad predictive-science environment of the center. Each student project entails scholarly goals commensurate with dissertation work that are motivated by specific center objectives. Most students were recruited into the center in its first year, shortly after joining Illinois. Three have, so far, completed internships at DOE/NNSA laboratories, with more internships being planned. Nick Christensen worked with Eric Parish at Sandia National Laboratories on parallel-in-time solvers; Shelby Lockhart worked with Carol Woodward and David Garner at LLNL on low synchronous orthogonalization in SUNDIALS; and Jacob Faibussowitsch worked with Will Pazner, Socratis Petrides and Rob Falgout at LLNL on matrix-free relaxation smoothers on GPUs.

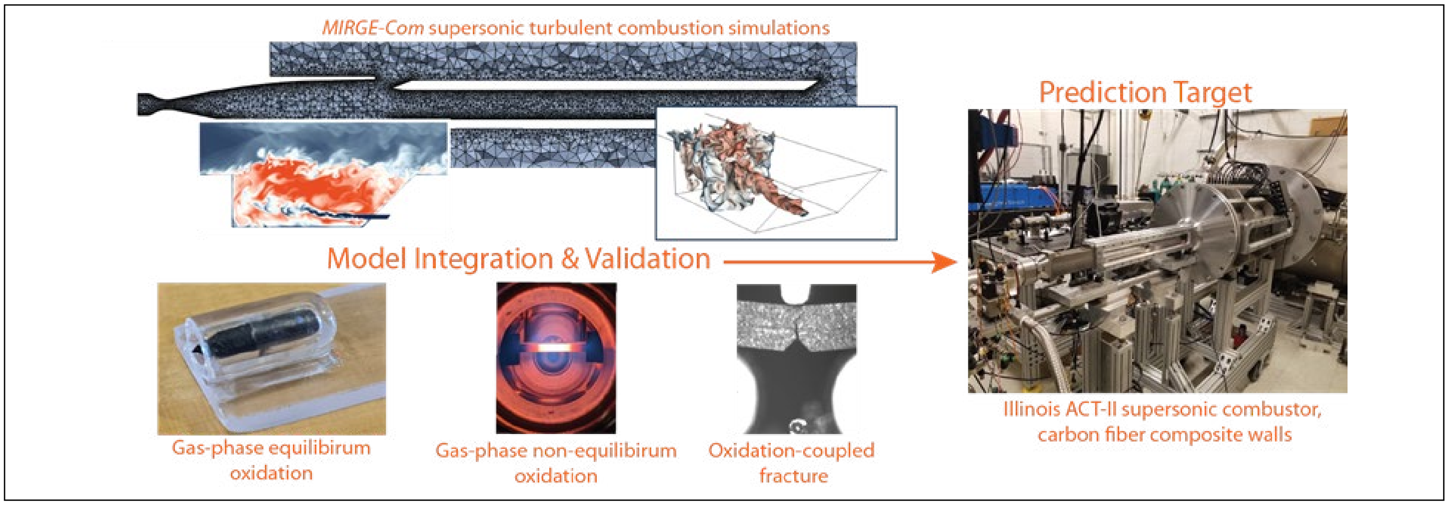


Figure 1. The CEESD prediction target is the temperature and degradation of a carbon fiber composite in the wall of the ACT-II supersonic combustion facility on the Illinois campus. Shown are example experiments this year, which map onto modeling objectives whose integration is essential to the overall prediction using our MIRGE-Com simulation tool.

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 focused 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, ultimately, uncertainty estimation particularly challenging.

The Center is a collaboration between research groups at the University of Maryland, the University of Southern California, and Massachusetts Institute of Technology.

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 is frequently 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 each other after some time. This linear instability also 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 from the bottom part of Figure 1, where the "noise" in the time-averaged QoI causes non-infinitesimal differences between parameter values that are infinitesimally close to each other.

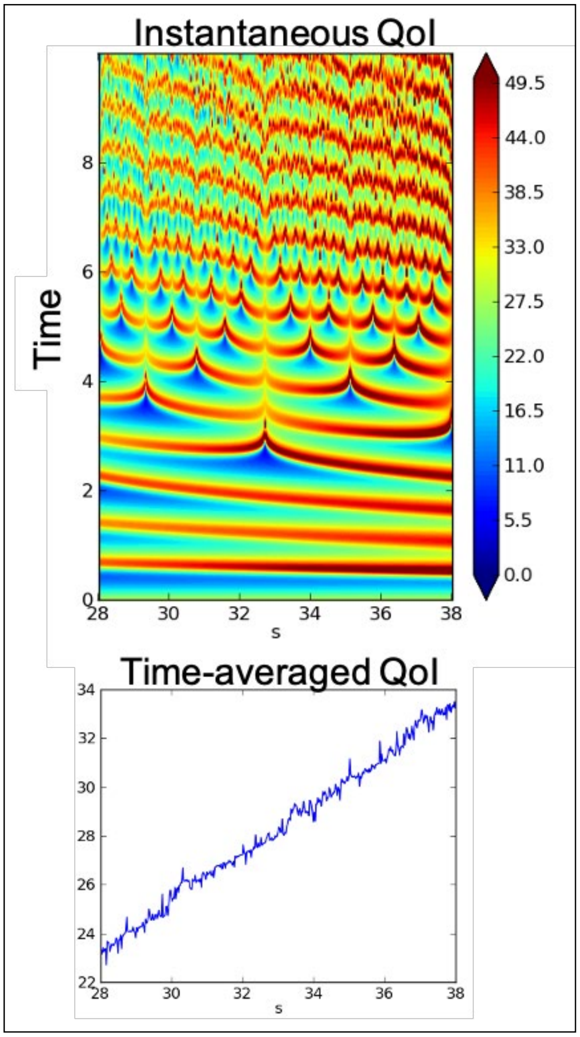


Figure 1. A sample Quantity-of-Interest (QoI) from the Lorenz system, illustrating the rapid de-correlation in time of nearby solutions (caused by differences in the parameters on the horizontal axis) which makes the problem of computing sensitivities of time-averaged QoIs an ill-posed problem (note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

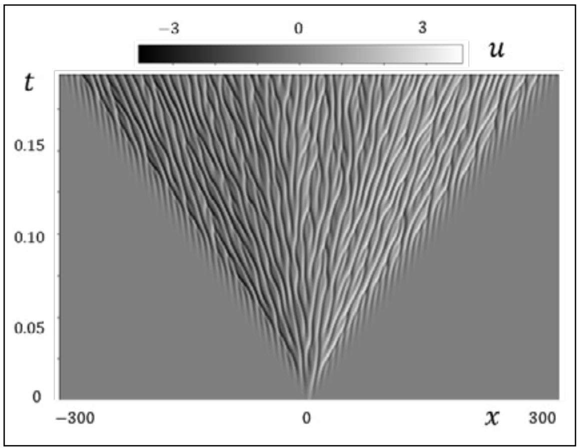


Figure 2. A solution to the Kuramoto-Sivashinsky partial differential equation which produces chaotic solutions in a low-dimensional context. This problem will be used in early assessments of the sensitivity estimation methods.

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 a joint benchmark problem. In addition to the main benchmark problem of turbulent flow, the Center also will consider problems like the Kuramoto-Sivashinsky equation (Figure 2). One approach will be to derive a mathematically-exact, regularized sensitivity and then 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 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. 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.

Evaluating the Performance-Portability of Irregular Halo Exchanges on National Nuclear Security Administration Applications

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

A key objective of the Center for Understandable Performant Exascale Communication Systems is understanding the communication performance of Department of Energy/National Nuclear Security Administration (DOE/NNSA) codes. As one initial study to understand irregular communication challenges, we examined communication in the CLAMR mini-application[1], followed by applying the insights from this study to the Los Alamos National Laboratory (LANL) Parthenon adaptive mesh refinement (AMR) framework. In particular, the goals of this initial study were to:

- Evaluate the performance of irregular halo exchanges
- Evaluate irregular communication performance of different message passing interface (MPI) implementations
- Understand the challenges new abstractions (e.g., neighbor collective application programming interfaces (APIs)) face for optimizing irregular halo exchanges.

Many applications and frameworks include an irregular communication primitive which exchanges a subset of one nodes' values with other nodes in the system. For example, CLAMR uses this primitive from the L7 library, the xRage production application uses a similar one, and both the Trilinos/Tpetra and Cabana frameworks implement this primitive in their respective Distributor classes.

MPI communication performance on irregular communication patterns, particularly in the face of load imbalance, varied significantly between MPI implementations and can reduce the performance of some codes by 25% or more. Figure 1 shows the performance difference of CLAMR with MVAPICH[2] and OpenMPI[3] on Quartz for the same input parameters. The difference in the execution times is in two functions (push_boundary and setup_comm) that use extensive MPI communication operations to exchange irregular halos between nodes.

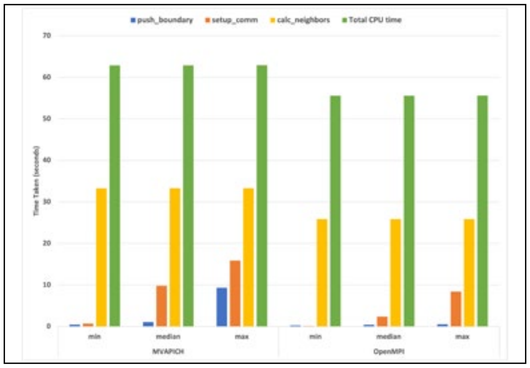


Figure 1. Performance on Quartz for CLAMR with two MPI implementations.

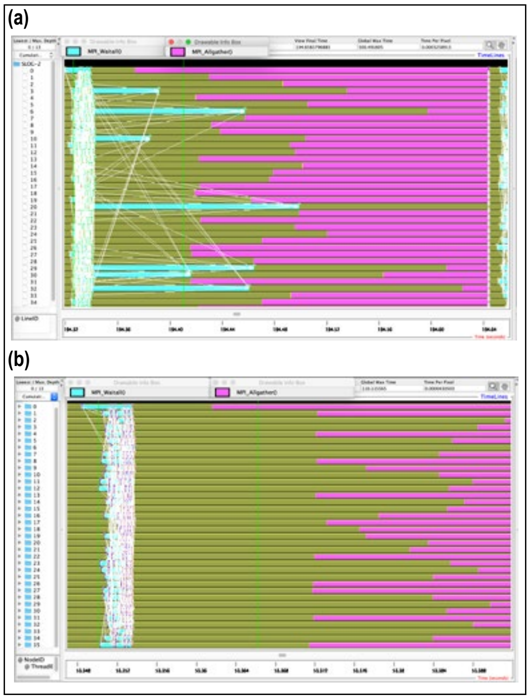


Figure 2. Process message-interactions for CLAMR (irregular halo exchanges and MPI_Allgather) for a 36-process/9-node problem case run on the LLNL Quartz system. Graphs show equal time elapsed on the X-axes. (a) CLAMR MVAPICH Traces. (b) CLAMR OpenMPI Traces.

Analyzing the sources of these differences, Figure 2 shows an equivalent duration of runtimes for the CLAMR mini-computational fluid dynamics (CFD) application with irregular halos running on the Lawrence Livermore National Laboratory (LLNL) Quartz system. These figures show that over the same time period, performance differs primarily as a result of poor message scheduling by the progress engine in the MVAPICH MPI implementation when using the shared memory transport between cores.

We then examined the communication performance of the Parthenon AMR framework[4] using a simple advection example. This study showed three main areas of communication: halo exchanges using persistent communication primitives, mesh block transfers using nonblocking sends and receives, and communicating the load balancing calculations (load costs) using MPI_Allgather. Significant time was spent within MPI_Wait during both halo exchanges and mesh block transfers, including processes with widely varying time in local calculations whose computation time was dependent on the number of the process's communication neighbors. This is thematically similar to CLAMR computation and communication behavior and highlights the potential importance of optimizing message scheduling for codes with large potential imbalances.

We drew these conclusions from this initial study:

- Performance of exascale halo codes depends strongly on details of production MPI implementations on leadership class systems.
- Application performance in the presence of weak progress is not predictable or performance-portable in current MPI implementations.
- Further examination and optimization of the communication behavior in imbalanced codes is an important future research area.

References

[1] D. Nicholaeff, et al., "Cell-based Adaptive Mesh Refinement Implemented with General Purpose Graphics Processing Units," 2011. Tech Report LA-UR-11-07127.

[2] D.K. Panda, et al., "The MVAPICH Project: Evolution and Sustainability of an Open Source Production Quality MPI library for HPC" in WSPPE (2013).

[3] E. Gabriel, et al., "Open MPI: Goals, Concept, and Design of a Next Generation MPI Implementation" in Proceedings of the 11th European PVM/MPI Users' Group Meeting, September 2004.

[4] Parthenon Performance Portable AMR Framework, 2021. Github: https://github.com/lanl/parthenon/wiki/Notes-on-Communication-Patterns.

Performance-Portable High Performance Computing with Python

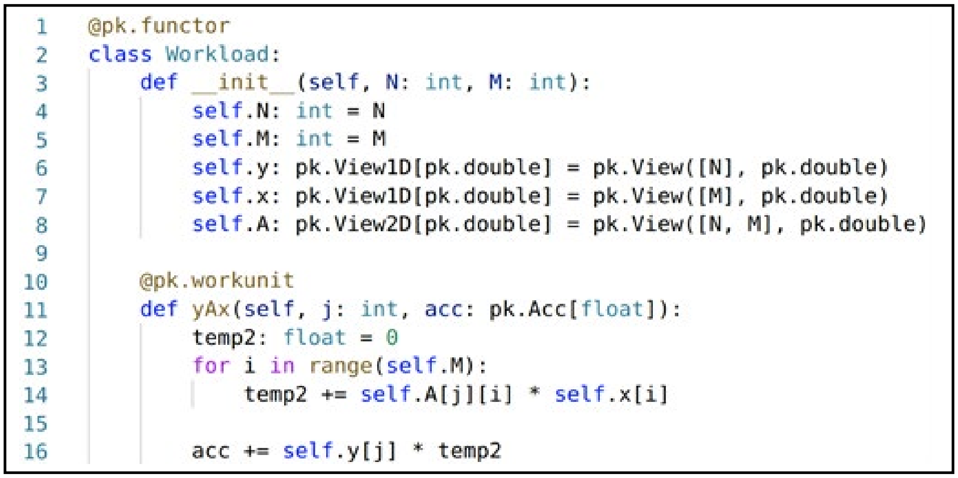
University of Texas at Austin ✦ PIs: Dr. Robert Moser (rmoser@oden.utexas.edu), Dr. George Biros (biros@oden.utexas.edu), and Dr. Milos Gligoric (gligoric@ece.utexas.edu); POC and Author: Nader Al Awar (nader.alawar@utexas.edu)

The current high performance computing (HPC) ecosystem is characterized primarily by heterogeneity in the hardware space. This presents a challenge to end users (i.e., scientists and programmers), as programming heterogeneous hardware requires learning different programming interfaces and optimal data layouts. Kokkos[1] is a programming framework that attempts to solve the challenge of heterogeneity through performance portability by providing a uniform programming interface and abstractions for data layouts on different hardware platforms—users can write their code once and run it on many different types of hardware. Kokkos is implemented using C++, a high-performance programming language seeing widespread use in HPC today.

Despite the advantages provided by C++, general usability remains an issue as the language is notorious for its steep learning curve. This is a significant problem in HPC, as many of the end users are scientists who lack formal training in computer science and software engineering. Instead of C++, scientists are likely to prefer languages such as Python, which emphasizes ease-of-use over other aspects (e.g., computational performance). Therefore, there is a need for an HPC framework that enables performance portability for Python users without sacrificing computational performance. The exascale computing team at the Predictive Engineering and Computational Science (PECOS) Center, therefore, has developed PyKokkos[2], a Python-based framework that enables scientists to write Kokkos-like applications entirely in Python.

The main goal of PyKokkos is to enable performance portable HPC in Python. PyKokkos improves on existing frameworks by having users write their code in Python and then transparently translates that code to C++ and Kokkos to achieve high performance.

Figure 1 shows an example code snippet written using PyKokkos that implements a matrix-weighted inner product kernel. PyKokkos first requires that users define a class marked with a specific decorator (line 1). This class also defines a constructor (lines 3-8), where the user defines member variables that will be used in the kernel.



```
1   @pk.functor
2   class Workload:
3       def __init__(self, N: int, M: int):
4           self.N: int = N
5           self.M: int = M
6           self.y: pk.View1D[pk.double] = pk.View([N], pk.double)
7           self.x: pk.View1D[pk.double] = pk.View([M], pk.double)
8           self.A: pk.View2D[pk.double] = pk.View([N, M], pk.double)
9
10      @pk.workunit
11      def yAx(self, j: int, acc: pk.Acc[float]):
12          temp2: float = 0
13          for i in range(self.M):
14              temp2 += self.A[j][i] * self.x[i]
15
16          acc += self.y[j] * temp2
```

Figure 1. An Example of a PyKokkos Code Snippet: Matrix-weighted inner product kernel.

These member variables must use type annotations (e.g., int, pk.View1D), as they will be used in code that is translated to C++. The user can then write their kernel in a method marked with another decorator (line 10). As before, type annotations are needed, because this method will be translated to C++. Crucially, the user does not need to interact with C++ at any point. PyKokkos will translate the kernel to C++ and then generate programming language bindings that connect the generated C++ with the user's Python code[2].

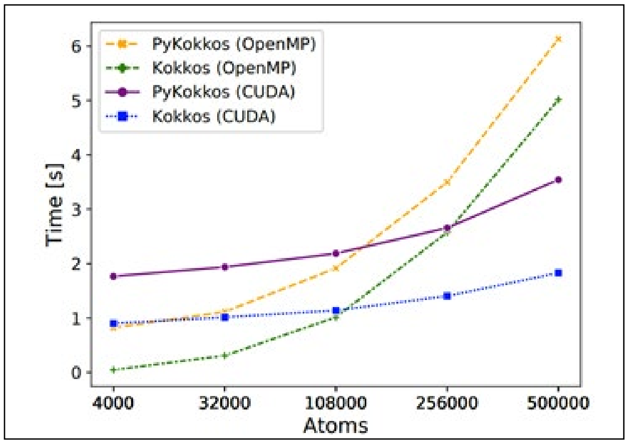


Figure 2. Simulation time (y-axis) for various number of atoms (x-axis) for ExaMiniMD.[3] PyKokkos time includes the startup of the Python interpreter which causes a slowdown.

PyKokkos was evaluated by migrating a large number of existing C++ and Kokkos scientific code to Python and PyKokkos[2], including ExaMiniMD[3] a molecular dynamics mini-app. Figure 2 shows plots comparing the PyKokkos and Kokkos implementations running on CUDA and OpenMP. The x-axis shows the input size, and the y-axis shows the execution time. The overhead introduced by PyKokkos is minimal and close to constant even as the input size increases. PyKokkos, therefore, is able to achieve its goals of ease-of-use combined with performance portability.

PyKokkos is being continuously extended and other large applications are being migrated from other large applications from C++/Kokkos to Python/PyKokkos. PyKokkos enables rapid prototyping (in Python) with good performance (by leveraging the Kokkos performance portability framework) which will have a substantial impact on science.

References

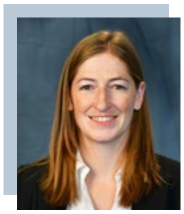
[1] C. Trott et al., "The Kokkos EcoSystem: Comprehensive Performance Portability for High Performance Computing," Computing in Science & Engineering 23, 5, pp. 10-18 (2021). DOI: 10.1109/MCSE.2021.3098509

[2] Nader Al Awar, Steven Zhu, George Biros, and Milos Gligoric, "A Performance Portability Framework for Python," Proceedings of the ACM International Conference on Supercomputing (ICS '21). Association for Computing Machinery, New York, NY, USA, 467–478 (2021). DOI: 10.1145/3447818.3460376

[3] ExaMiniMD (2027). https://github.com/ECP-copa/ExaMiniMD.

Abigail Hunter, Los Alamos National Laboratory (ahunter@lanl.gov)

Years at Lab: 2011-Present, **Degree:** PhD, Mechanical Engineering ✦ **PSAAP Program:** 2008-2011, Purdue University



My graduate school research was focused on using mesoscale modeling approaches to study the motion and interaction of dislocations in metals. This work was supported by one of the first Predictive Science Academic Alliance Program (PSAAP) centers, specifically the Center for Prediction of Reliability, Integrity, and Survivability of Microsystems (PRISM) at Purdue University. My ongoing work at Los Alamos National Laboratory (LANL) is built on this foundation. Currently, I focus on the development and use of models that describe material strength and the evolution of damage in metals at both the meso- and macro-scales under a wide range of loading conditions. In particular, I have specific interest in connections between microstructure, dislocation-based deformation behaviors, and overall material response.

PSAAP gave me the unique opportunity to visit and work at LANL for an extended period of time during graduate school. While the program promotes a 10-12 week visit for students, my academic advisor and LANL mentors allowed me to stay for almost 6 months. This gave me the opportunity to fully experience life at the laboratory and to meet and interact with many scientists. During this time, I also was able to interview for postdoctoral positions at LANL. Once I started as a postdoctoral research associate, I was provided opportunities to expand the interests and expertise I developed in graduate school to include macro-scale model development to predict strength and damage in metals under a wide range of loading conditions, including extreme loading conditions such as shock loading. This foundation has contributed to many successes I have achieved thus far in my career, including recently receiving the Presidential Early Career Award for Scientists and Engineers (PECASE) in 2019 for work developing and implementing models addressing brittle damage and dislocation dynamics in metals, in addition to science, technology, engineering, and mathematics (STEM) outreach efforts.

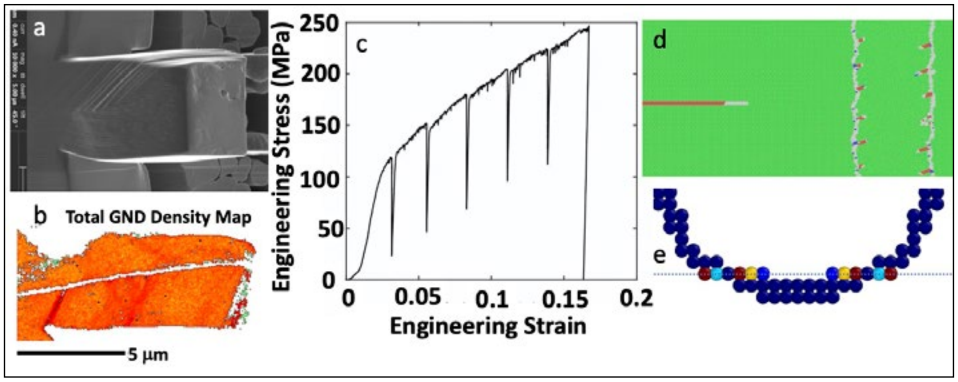


Figure 1. Dr. Hunter is the PI (with S. Fensin, co-PI) of an Laboratory Directed Research and Development project entitled ‘Investigating How Material’s Interfaces and Dislocations Affect Strength (iMIDAS)’. This project is developing an integrated approach allowing for the investigation of the role that grain boundary structure and dislocation grain boundary interactions play in overall mechanical response (Figure c). State-of-the-art experiments (Figures a, b, c) using *in situ* scanning electron microscopy (SEM) and high resolution electron backscatter diffraction (EBSD) can image lattice rotations and the evolution of geometrically-necessary dislocations (Figure b) correlated with dislocation-grain boundary interactions in bicrystal micro-pillars (Figure a). Similar boundaries can then be modeled using atomistic (Figure d), meso-scale (Figure e), and macroscale (not shown) simulation techniques. Figures courtesy of Nan Li, Jonathan Gigax, Dongyue Xie, Saryu Fensin, Sumit Suresh, Xiaoyao Peng, Nithin Mathew, D.J. Luscher.

> *“While the program promotes a 10-12 week visit for students, my academic advisor and LANL mentors allowed me to stay for almost 6 months. This gave me the opportunity to fully experience life at the laboratory and to meet and interact with many scientists.”*

Overall, I believe that one of the most attractive features of the Department of Energy/National Nuclear Security Administration national laboratories is the wide breadth of science and engineering investigated at these institutions. This aspect of the national laboratories was one of the most compelling features to me and was one of the primary reasons that I wanted to work at LANL. As someone who primarily works on the development of computational models, the impressive experimental facilities and being able to easily collaborate with experimentalists is extremely valuable for developing reliable, validated models. Additionally, the diverse work completed at LANL allows for so many possibilities for future collaborations and the ability to address novel, cutting-edge research questions.

Benjamin J. Isaac, Lawrence Livermore National Laboratory (isaac4@llnl.gov)

Years at LLNL: 2014-2019, **Degree:** PhD, Chemical Engineering and Engineering Sciences ✦ **PSAPP:** 2014-2019, University of Utah

I The Predictive Science Academic Alliance Program II (PSAAP II) supported my research for several years as a research associate under the direction of Dr. Philip J. Smith at the University of Utah. The research within our multidisciplinary simulation center was focused on the simulation of pulverized coal combustion in industrial-scale power boilers. The multi-physics involved in simulating these systems is complicated and couples several areas of study such as: fluid mechanics, radiation transport, chemistry, particle transport, and material science. My research focused on developing a heterogenous chemistry treatment for the reaction of the coal particles, implementing particle transport methods, and creating models to treat the complex, thermal boundary environments on the boiler walls. In our efforts to quantify our ability to predict the behavior of these industrial scale systems I was introduced to the field of uncertainty quantification. PSAAP II facilitated a visit for one week at both Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory (LLNL) where I was able to collaborate with staff scientists on implementing an alternative Large Eddy Simulation closure which we used in some of our boiler simulations. These visits helped me draw several connections between my work at the center and the work being done at the lab. The visits also provided networking opportunities and ultimately sold me on the career opportunities provided by Department of Energy/National Nuclear Security Administration's (DOE/NNSA) national laboratories.

In 2019, I was hired by the Design Physics division at LLNL as a computational physicist. My position focuses on the continued development of LLNL's ALE3D code which encompasses a wide range of physics and capabilities. This allows me to work on some familiar problems involving chemistry and radiation, as well as some new topics. In addition, I have been able to learn and participate in code porting activities to enable our software to take advantage of graphics-processing-unit-accelerated platforms.

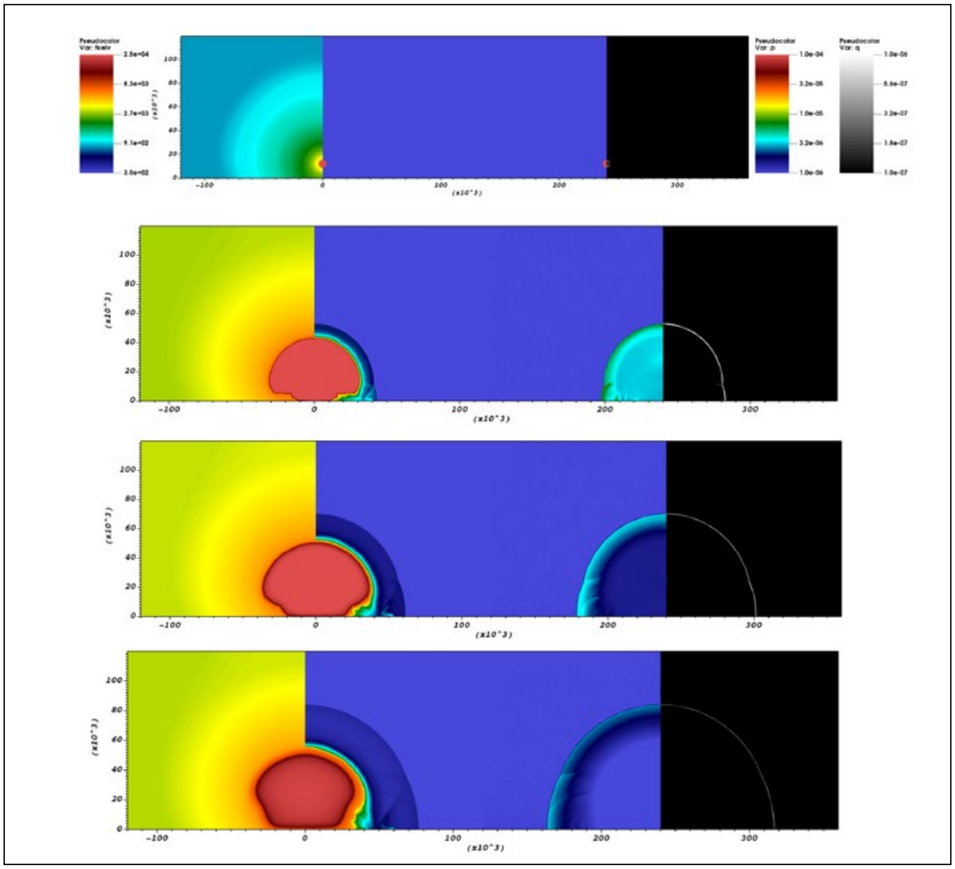


Figure 1. In one of my projects, we are working on developing tools to be able to better predict the post nuclear detonation environment. In this project I was responsible for incorporating appropriate thermal radiation models and adding coupling terms to explicit hydrodynamics. The complex heating, cooling, mixing, and chemistry occurring in this system all play a role in predicting the evolution of fallout material. Here we show an ALE3D calculation[1] of an idealized 100 KT near surface detonation. The four snapshots in time (a: 0.25 ms, b: 0.25 s, c: 0.5 s, and d: 1.0 s) show the radiation and matter temperature, pressure, and artificial viscosity (from left to right).

> *“PSAAP II facilitated a visit for one week at both Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory (LLNL) where I was able to collaborate with staff scientists on implementing an alternative Large Eddy Simulation closure which we used in some of our boiler simulations.”*

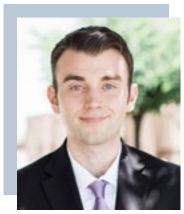
Being able to work at LLNL has provided opportunities that are unique to NNSA's national laboratories. All my projects are focused on solving grand challenge problems of national interest. Due to the nature of the lab's work, I have access to some of the world's largest super computers. As an LLNL employee my continued education and training has come at the hands of leading scientists in their respective fields.

Reference

[1] A. Shestakov, A. Nichols, B. Isaac, J. Morris, & K. Knight, "Challenges in Simulating Ground Interacting Nuclear Explosions" (No. LLNL-JRNL-814197) (2020). Lawrence Livermore National Lab. (LLNL), Livermore, CA (United States).

David Zwick, Sandia National Laboratories, (dzwick@sandia.gov)

Years at SNL: 2019-Present, **Degree:** PhD, Mechanical Engineering ✦ **PSAAP:** 2015-2019, University of Florida



I am an application software developer of a physics code called Lagrangian Grid Reconnection (LGR - pronounced "logger"). Although there are many physics codes across the Department of Energy/National Nuclear Security Administration (DOE/NNSA) laboratories, LGR's claim-to-fame is its ability to simulate magnetohydrodynamic problems of interest on modern high-performance graphics-processing-unit (GPU)-based systems. It does this by using novel numerical methods and the latest advances in computer science. As a developer, my day-to-day work is equally challenging and rewarding. One of the best benefits of working at Sandia National Laboratories (Sandia) is that I am surrounded by other talented and driven experts who continually push the boundaries of what is possible in the national security arena. Additionally, since LGR is a production software, I often interact with a variety of both internal and external customers who each have unique needs. I find it especially rewarding when I can incorporate a new feature or technique within the software that greatly improves their experience.

Whereas my decision to join Sandia was undoubtedly a great one, it wasn't always as clear. In fact, when I first began my PhD program at a Predictive Science Academic Alliance Program (PSAAP) center I wanted to become a professor. This was, in part, because I thought that there were only two technical tracks: industry or academia. I never knew that there could be a third option at a national laboratory which shares the best aspects of both. However, the PSAAP program helped me determine that a national laboratory would be a great fit. Through the PSAAP's required internship program, I was able to see what it was like to perform research and development in a national laboratory setting. During my tenure, I also gained skills through different experiences that I directly applied to my current job, which included technical presentation experience and even supercomputing training and resources. Additionally, the tuition assistance I received from the program helped me to focus on my research and not on finding additional funding.

When I completed my degree, it was clear to me from my time at my PSAAP center that I wanted to work for an DOE/NNSA laboratory. I am happy to say that after completing my first two years at Sandia, I am not only pleased with my decision but also am proud to be a Sandian.

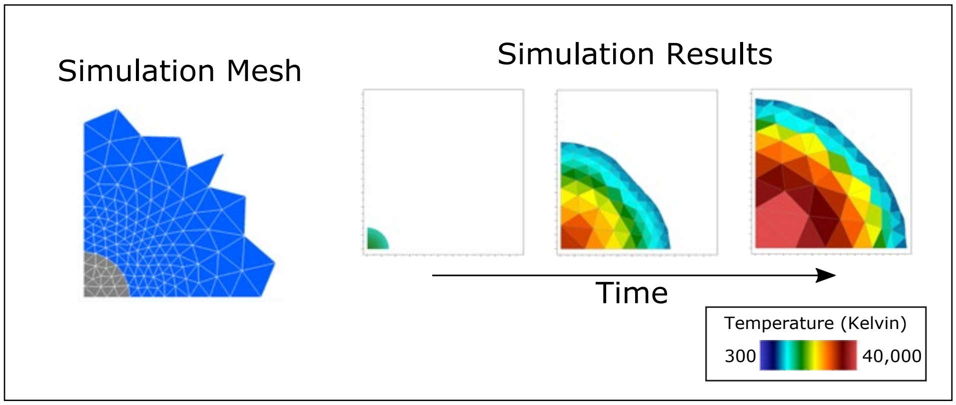
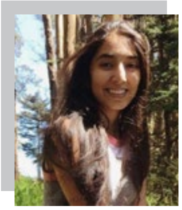


Figure 1. An example of one of LGR's simulation output is shown in Figure 1. Figure 1 shows a model of a quarter cylinder expanding, as it is rapidly heated. The contours from the simulations provide insight into the physics that cannot be attained through other experiments.

> *"...when I first began my PhD program at a Predictive Science Academic Alliance Program (PSAAP) center I wanted to become a professor. This was, in part, because I thought that there were only two technical tracks: industry or academia. I never knew that there could be a third option at a national laboratory which shares the best aspects of both. However, the PSAAP program helped me determine that a national laboratory would be a great fit."*

Purvi Goel (pgoel2@stanford.edu)

Degree in Progress: PhD, Computer Science, Stanford University ✦ **Advisor:** Dr. Doug L. James ✦ **PSAAP:** 2019-Present

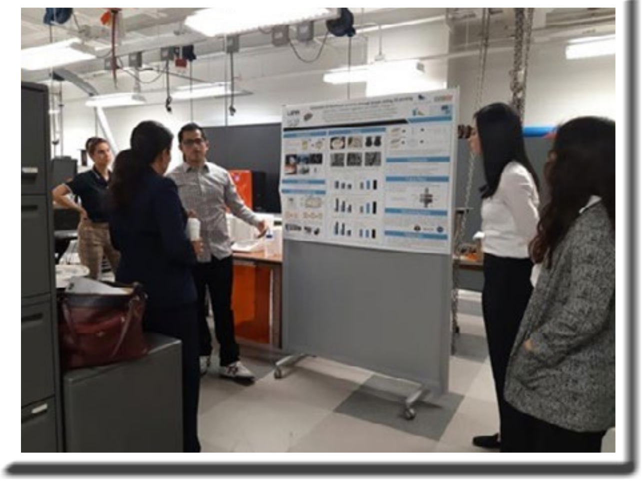


Powered by exascale supercomputers, Stanford's Integrated Simulations using Exascale Multiphysics Ensembles (INSIEME) Predictive Science Academic Alliance Program III (PSAAP-III) Center's rocket ignition simulation ensembles will range in size from hundreds to millions of samples and will characterize the effect of design choices and input uncertainties when assessing the reliability of the LOX-CH4 ignition process. Unfortunately, users cannot easily inspect or compare specific ignition outcomes, such as success versus failure, due to data overload. But in order to understand, compare, and gain insights within the design space of simulation input parameters, a user should be able to see and directly manipulate a rich record of ensemble data. A better understanding of the relationships between simulation inputs (e.g., combustion chamber length), initial chamber chemistry, and domain temperature and outputs can empower more informed steering of the ignition ensemble and identification of important events in the ignition process.

My focus in the Center is building a query-based ensemble exploration tool that enables users to browse exascale simulation output data flexibly (users can navigate the high-dimensional search space in a variety of ways) and efficiently (users can explore ensemble data at interactive rates). To support these goals, I am developing novel data structures optimized for evaluating spatiotemporal user queries, methods to summarize ensemble samples, and generate lightweight-but-expressive, in-core representations that can be rapidly explored and visualized using our browser interface.

Working in Stanford's INSIEME PSAAP-III Center gives me the opportunity to work with powerful exascale solvers producing vast amounts of simulation data (i.e., terabytes). The sheer amount of computing power to which we have access within our PSAAP-III Center allows the team to conduct more ambitious designs of experiments and to cultivate larger ensembles. Ensembles of this sample size, resolution, and richness are a rare and valuable commodity for data analysis. These large ensemble sizes, particularly at exascale, both necessitate novel browsing tools for analyzing and exploring the enormous amounts of output data and motivates my interest in ensemble exploration. In addition, the PSAAP-III project allows me to work closely with an interdisciplinary team of world-class researchers. Their direct experience with the rocket-ignition ensembles that we hope to explore, the selection of meaningful simulation parameters to navigate high-dimensional search spaces, and on-data analytics questions within multiphysics ensembles makes their feedback indispensable, as I invent exciting new browsing technologies.

Minority Serving Institutions Partnership Program



Overview

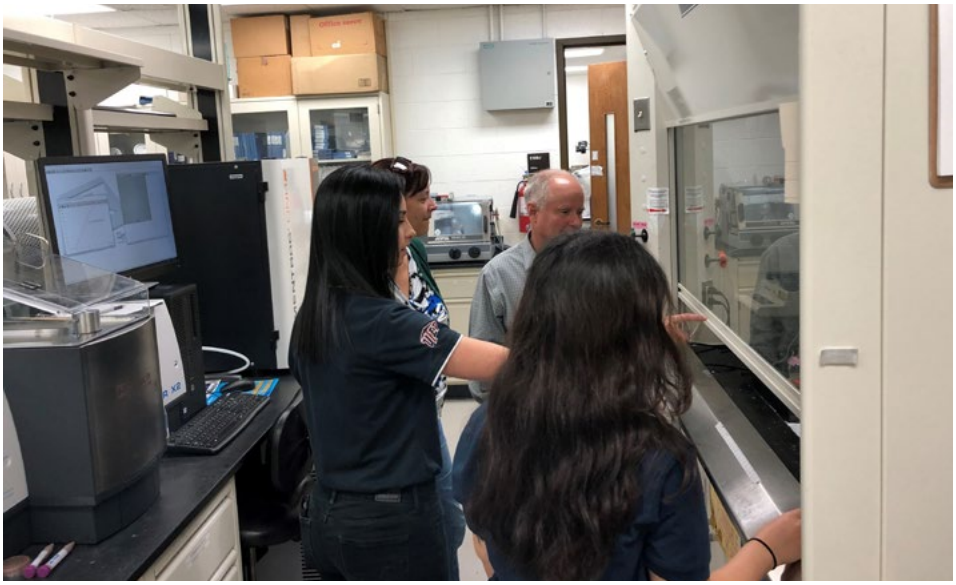
Dr. Beatriz Cuartas, Federal Program Interim Director (MSIPPReports@nnsa.doe.gov) ✦ National Nuclear Security Administration

The Minority Serving Institutions Partnership Program (MSIPP) and Tribal Education Partnership Program (TEPP) award grants to Minority Serving Institutions (MSI), who partner with national laboratories and plants, to prepare a diverse, sustainable, and highly skilled pipeline to fill NNSA's DEIA succession planning gaps with top science, technology, engineering, and mathematics (STEM) talent to be the next-generation workforce that looks like America.

MSIPP/TEPP continue to drive towards NNSA's Strategic Vision Mission Priority #4 to strengthen key STEM capabilities through its enduring STEM networks of MSIs, and M&O partners supporting research and students ranging from K-12 to the postdoctoral level.

Funding for the program is identified in the National Defense Authorization Act. In FY22 MSIPP/TEPP appropriations amounted to $50 million. Since 2019, the funding for the program has increased by 125 percent, and has resulted in the program increasing partnerships by 300 percent (6 consortia in 2019 to 24 consortia with 46 schools in FY21).

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 Indian Higher Education Consortium, Lead
- Advanced Sensors Technologies for Applications in Electrical Engineering - Research and Innovation excellence Consortium (ASTERIX), Florida International University, Lead
- Advanced Synergistic Program for Indigenous Research in Engineering (ASPIRE), Turtle Mountain Community College, Lead
- Application of Artificial Intelligence to Cybersecurity for Protecting National Critical Infrastructure (CONCISE), The University of Texas at San Antonio, Lead
- Consortium of Advanced Additive Manufacturing Research and Education for Energy Related Systems (CA2REERs), The University of Texas Rio Grande Valley, Lead
- Consortium enabling In- and Ex-Situ-Quality Control of Additive Manufacturing (QCAM), New Mexico State University, Lead
- Consortium for High Energy Density Science 2.0 (CfHEDS-2), Florida A&M University, Lead
- Consortium for Laser-based Analysis of Nuclear and Environmental Materials (LANEM), Florida A&M University, Lead
- Consortium for Research and Education in Materials Science and Photonics Engineering (NoVel), Norfolk State University, Lead
- Consortium for Research and Education in Power and Energy Systems (CREPES), Florida International University, Lead
- Consortium for Nuclear Security Advanced Manufacturing Enhanced by Machine Learning (NSAM-ML), North Carolina Central University, Lead
- Consortium Hybrid Resilient Energy Systems (CHRES), Sistema Universitario Ana G. Mendez, Incorporado, Lead
- Consortium on Nuclear Security Technologies (CONNECT), The University of Texas at San Antonio
- Energy Sciences: Experimental and Modeling Consortium (ESEM), Prairie View A&M University, Lead
- Growing STEMs Consortium: Training the Next Generation of Engineers for the DOE/NNSA Workforce (GSC), Texas Tech University System, Lead
- Integrated Additive Manufacturing – Establishing Minority Pathways: Opportunities for Workforce-development in Energy Research and Education (IAM-EMPOWEREd), Florida A&M University, Lead
- Nuclear Security Science and Technology Consortium (NSSTC), University of Nevada Las Vegas, Lead
- Partnership for Advanced Manufacturing Education and Research (PAMER), Navajo Technical University, Lead
- Partnership for Proactive Cybersecurity Training (PACT), The University of Arizona, Lead

- Partnership for Research and Education Consortium in Ceramics and Polymers 2.0 (PRE-CCAP-2), University of Texas at El Paso, Lead
- Pipeline Development of Skilled Workforce in STEM through Advanced Manufacturing (STEAM), North Carolina A&T University, Lead
- Scholarly Partnership in Nuclear Security (SPINS), Alabama A&M University, Lead
- Successful Training and Effective Pipelines to National Laboratories with STEM Core (STEP2NLs), North Carolina A&T 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

For more information, visit https://orise.orau.gov/NNSA-MSIIP/.

Joseph Bell, Y-12 National Security Complex

Years at Y-12: 2015-2021 ✦ **Degree:** PhD, Physics ✦ **MSIPP:** 2019-2020, Fisk University

Research Topic

Ceramic Neutron Detection Material

Figure 1. Joseph Bell conducting research in the lab while attending Fisk Vanderbilt Bridge on senor devices.

> *This partnership between MSIPP and Y-12 combined with the ability to work with highly skilled scientists and engineers, afforded me the opportunity to obtain my masters and doctorate at Fisk University and Vanderbilt University, respectively.*

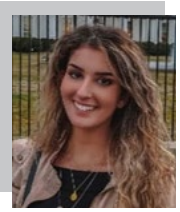
The Minority Serving Institution Partnership Program (MSIPP) has played a key role in my academic and professional development by allowing me to intern at Y-12 National Security Complex. As a Y-12 summer intern for the past six years, I have become highly acquainted with both the national security complex and lithium-based crystals and ceramic research. This partnership between MSIPP and Y-12 combined with the ability to work with highly skilled scientist and engineers, afforded me the opportunity to obtain my master's and doctorate at Fisk University and Vanderbilt University respectively.

During my tenure as a student, I gained the skills necessary to become a reputable scientist in both an academic and government setting. My graduate research involved the growth and characterization of radiation detecting crystals and ceramics. I mastered the ability to grow scintillating and semiconducting crystals and ceramics for use as radiation detectors. This led to numerous publications, conference presentations and, most importantly, a masters and PhD in physics.

My professional career also flourished because of this partnership. Working side-by-side with scientists and engineers at Y-12, I have forged key relationships and accomplished research objectives which align with the goals of Y12's lithium operations department and ceramic work. This work allowed me to seamlessly transition from an intern to a full-time employee. Because the MSIPP made this opportunity possible, I am trusted to lead my own project to further the goals of Y-12 while being in a position to help other students advance their academic and professional careers.

Ava Benkhatar

Degree in Progress: PhD, Physics, University of Nevada, Reno ✦ **Advisor:** Dr. Roberto C. Mancini ✦ **MSIPP:** 2019-2022



Research Topic

Social Sciences - Political Science

Research Responsibilities

My main research responsibility for my most recent Minority Serving Institutions Partnership Program (MSIPP) internship year was to support the Lawrence Livermore National Laboratory (LLNL) radiological security program in assessing and developing training materials for foreign partners. During my time as an intern I also supported ongoing research and data gathering activities to identify trends in irradiator research over time to help inform program strategy development.

Benefits of MSIPP

I have greatly benefited from the MSIPP internship! This internship has provided me with opportunities that have supplemented my academic research, networking abilities, and my career prospects. Through interning at LLNL for the previous two years of my MSIPP internship, I have learned a lot about the lab's mission and established meaningful relationships with the mentors and faculty members I've worked with throughout the years. Each seminar that was presented through the MISPP internship gave me insight that I feel helped me improve personally and professionally. With this internship I was able to conduct research that was relevant to the focus areas of my degree as well as see what occupations in my prospective field look like. Most significantly, MSIPP's network provided me with the opportunity to apply for (and secure) a government position immediately after graduation.

New Contacts, New Opportunities

MSIPP absolutely gave me the opportunity to work with others I might not have otherwise. During my second year as an undergraduate student, I applied to the MSIPP internship for the first time after a professor had recommended it to me. The program's mission and scope aligned with my interests and I was very impressed with the large selection of labs and headquarters they collaborated with. I found out that I had been selected for the program around the same time that the pandemic started so I was incredibly relieved that MSIPP decided to go-on with the program and offer it virtually. MSIPP's decision to offer a virtual internship gave me the opportunity to continue to supplement my degree and academic research at a time when so many others couldn't. Through offering a virtual internship I was not only able to receive the full internship experience, but I was also offered an extension that lasted until the end of the year so that I would be able to complete my project. This extension allowed me to collaborate with faculty members outside of the internships network and work with researchers and professionals from other departments that were conducting research with a similar focus. This was an especially beneficial opportunity for me as I was able to establish a closer relationship with the lab's program-software and tech teams. These relationships helped me become more familiar with the different types of technology and software I was using to conduct my research and, thus, greatly expanded my technological skill set. With the knowledge I obtained through my collaboration with the LLNL's technology team and my previous mentors, I was able to rejoin MISPP the following year.

My second year as a MSIPP intern was especially important, as it gave me the opportunity to work with professionals in my prospective career during the final semester of my undergraduate degree. Being able to conduct research on nuclear irradiators and nuclear policies with established scientists and field experts provided me with relevant career experience and a strong network of professional connections. That experience and those connections ultimately led to me being recommended for a Program Manager position at the University of California, Berkeley by a mentor I worked closely with at LLNL. Upon looking into the position and interviewing for it, I was offered the job. This position alone has opened up a world of opportunities for me and would not have been possible without MSIPP and its incredible network of researchers, mentors, and career professionals.

Minority Serving Institutions Partnership Program

The Department of Energy/National Nuclear Security Administration (DOE/NNSA) has a vital national security mission to protect the American people by maintaining a safe, secure, and effective nuclear weapons stockpile. This mission could not be accomplished without MSIPP/TEEP's focus on building a Science, Technology, Engineering and Mathematics (STEM) succession strategy to build capacity, drive innovation, and ensure we have a world class workforce that looks like America to meet the security demands of the present and future federal workforce.

As quoted from the White House's report, *Charting A Course For Success: America's Strategy for STEM Education*, "The pace of innovation is accelerating globally, and with it the competition for scientific and technical talent. Now more than ever the innovation capacity of the United States—and its prosperity and security—depends on an effective and inclusive STEM education ecosystem."

For more information, please visit our website: NNSA Minority Serving Institution Partnership Program (MSIPP) | Department of Energy

Caption for Photo on MSIPP Section Page

UTEP PRE-CCAP students presenting research project to Dr. Beatriz Cuartas (MSIPP Acting Director). From Left to right, Paulina Ibave (currently full time at Microsoft), Dr. Beatriz Cuartas, Luis Chavez (currently full time at LANL), Bethany Wilburn (currently full time at KCNSC), and Elizabeth Reza (currently full time at KCNSC).

Fellowship Programs

Andrew Stershic, Sandia National Laboratories (ajsters@sandia.gov)

Years at SNL: 2016-Present ✦ **Degree:** PhD, Civil and Environmental Engineering, Duke University ✦ **CSGF:** 2012-2016

The Department of Energy (DOE) Computational Science Graduate Fellowship (CSGF) was a unique opportunity during graduate school that opened doors for me in the field of computational science. The demanding, yet rewarding, combination of educational training, professional networking, and national laboratory internship helped me to develop skillsets essential for the national laboratory system.

During the second year of my PhD at Duke University, I participated in a practicum at Oak Ridge National Laboratory (ORNL). I spent the summer researching a wide range of topics, from ballistic impacts in sand to lithium-ion battery cathode microstructure. The discrete element method (DEM) approach that I used to model the cathode microstructure lends itself well to parallel computing, allowing me to run highly-resolved simulations daily on ORNL's High Performance Computing (HPC) clusters. Sitting one floor beneath my office, ORNL's Titan supercomputer was ranked first globally at the time for computational power. This formative experience helped me to broaden my technical expertise, make connections with career scientists, and explore the verdant hills and refreshing swimming holes of the Cumberland Plateau.

The technical expertise I gained through graduate school and the CSGF internship, as well as the professional networks, led me to my current position as a mechanical engineer at Sandia National Laboratories. In this role, I develop research and apply it to solve our national security challenges, mirroring the role of the national laboratory system as a whole. Specifically, I focus on improving computational modeling of material failure by developing novel fracture modeling approaches for finite element analysis. These new approaches address a decades-old challenge in fracture modeling: the most commonly used models do not converge with finite element mesh refinement. Overcoming this obstacle means that it is easier to trust modeling and simulation predictions for Sandia's mission-driven failure and safety analyses. Partnering with scientists in the physical laboratories at Sandia allows our team to demonstrate and validate these models against test data from representative problems (Figure 1).

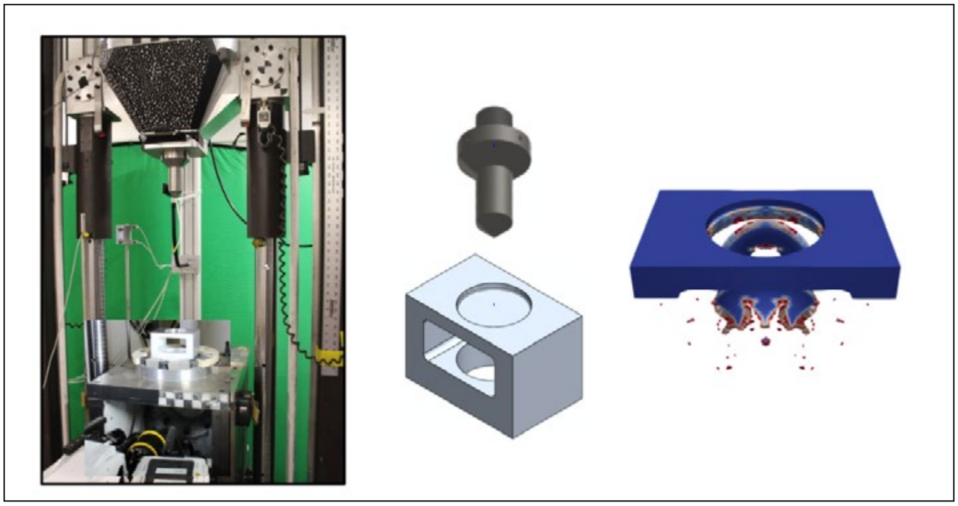


Figure 1. Laboratory puncture testing of an aluminum specimen, using a gravity-driven punch. Experiment results are used for validation of new failure modeling capabilities. Photo Credit: S. Kramer, SNL

> *"The technical expertise I gained through graduate school and the CSGF internship, as well as the professional networks, led me to my current position as a mechanical engineer at Sandia National Laboratories."*

In addition to building on my graduate expertise in fracture modeling, my experience at Sandia has allowed me to work in diverse areas ranging from structural safety analyses of laboratory testing facilities to simulation of manufacturing processes (e.g., forging, machining, welding) to predict residual stresses in metallic components.

As my career at Sandia has matured, I have grown my network and connected to other government institutions and universities to strengthen my research and to maximize its impact. This includes partnering with manufacturing analysts at the DOE/National Nuclear Security Administration's (DOE/NNSA's) Kansas City National Security Campus and munitions engineers at the Army Research Laboratory and the Air Force Research Laboratories through the Department of Defense (DoD)-DOE Joint Munitions Program. I have maintained relationships with my alma mater, Duke University (PI: J. Dolbow) for failure modeling and have fostered new ones with the University of California, Davis (PI: M. Hill) to leverage their extensive residual stress measurement capability.

The CSGF showed me the value of having good mentors. As an established staff member at Sandia, I have an opportunity to mentor others and attract talent to the national laboratory system. I serve as CSGF practicum coordinator for the Sandia-Livermore site in California, coordinating internships for CSGF fellows and potentially for careers with Sandia. I regularly have the opportunity to mentor summer interns and new staff-members within our department. Reflecting on my CSGF experience, I'm grateful for the networks and practical experiences that helped catalyze my career in the national laboratories.

Samuel Olivier, University of California, Berkeley (soliver@berkeley.edu)

Degree in Progress: PhD, Applied Science and Technology ✦ **Advisor:** Dr. Rachel Slaybaugh ✦ **CSGF:** 2018-Present

Research Topic

High-Order Variable Eddington Factor Methods for Thermal Radiative Transfer

Research Responsibilities

I work closely with Lawrence Livermore National Laboratory (LLNL) on a Laboratory Directed Research and Development (LDRD) project to develop high-order, finite element methods for thermal radiative transfer (TRT). TRT is a crucial form of energy transfer in high energy density physics experiments conducted at facilities such as the National Ignition Facility (NIF). There, the world's most powerful laser heats a gold cylinder to millions of degrees resulting in the release of thermal X-rays that bathe a BB-sized capsule filled with isotopes of hydrogen. The X-rays burn the capsule, compressing the hydrogen plasma inside enough to fuse nuclei.

Predictive models of NIF require the accurate modeling of the release, movement, and deposition of this radiative energy. Fully describing radiation requires a seven-dimensional phase space that defines an X-ray's position in space and time and the direction and frequency with which it is traveling. This large phase space means that models of radiation have orders of magnitude more computational work and memory requirements than other aspects of a NIF simulation such as fluid dynamics.

My research aims to reduce this cost by developing new algorithms that take advantage of the physics of the problem and emerging computer architectures. In particular, I have developed Variable Eddington Factor (VEF) methods that iteratively couple the transport equation to its moments. This moment-based approach reduces cost by coupling the lower-dimensional moments to the other physics components in the simulation in place of the expensive transport equation. The primary contribution of my thesis work is the development of VEF methods that are compatible with the high-order, finite element methods used at LLNL that can be efficiently solved using existing preconditioned iterative solvers. These methods currently are being implemented in LLNL's next-generation TRT code.

Benefits of CSGF

My research would not have been possible without the Computational Science Graduate Fellowship (CSGF). CSGF's financial support has allowed me to work exclusively on projects about which I am passionate and have enabled fruitful collaborations at both the laboratories and in academia. The course requirements in the Program of Study encouraged me to branch out, develop new skills, and, ultimately, paved the path toward success in my research. Finally, CSGF supported three summer practicums (two at LLNL, one at Los Alamos National Laboratory) which gave me my research topic, the purpose to pursue it, access to computational tools, and, most importantly, mentorship from staff at the labs.

Jesse A. Rodriguez, Stanford University (jrodrig@stanford.edu)

Degree in Progress: PhD, Mechanical Engineering ✦ Advisor: Dr. Mark A. Cappelli ✦ **CSGF:** 2018-2021

Research Topic

Reconfigurable Plasma Metamaterial Devices for Optical Computing Applications

Research Responsibilities

In my lab, I help lead our investigation into reconfigurable plasma metamaterial devices, particularly those created using inverse design (machine learning) methods. At the moment, we are carrying out investigations in three major areas. One is in plasma metamaterials with magnetized plasma elements. This area is in the stage at which we are pursuing fundamental physics results to see if the individual elements of our devices will behave as we expect. Another area is theoretical inverse design of plasma metamaterials where we use machine learning in tandem with finite difference frequency domain simulations of Maxwell's equations to come up with novel optical devices. Finally, in our third area, we are working toward translating these simulated devices into laboratory experiments, primarily using novel, tunable plasma elements that have a robust mapping between input parameters and plasma density.

Benefits of CSGF

Of course, with any very generous external reward like the Computational Science Graduate Fellowship (CSGF), this funding has allowed me to dictate my own path through the PhD program here at Stanford with freedom to choose both my own research topics and my own course load to optimize my training. Beyond this and more unique to the CSGF, having this particular fellowship has pushed me to pursue significantly more training in computer science than I otherwise would have which has been an incredible boon to my research. In addition, I would be remiss to not mention how great it was to spend a summer working with Princeton Plasma Physics Laboratory (PPPL) for my practicum. That experience was my first opportunity to work with world-class high performance computing (HPC) resources, and it has long been a dream of mine to work on the cutting edge of fusion research which is exactly where the Fusion Recurrent Neural Network (FRNN) team at PPPL operates.

What Students Considering CSGF Should Know

The main thing that comes to mind is that I would encourage students to apply for the CSGF regardless of their computing background going into their doctoral program. I had very little scientific computing background prior to graduate school, but I made sure to express in my fellowship application that I had a strong interest in utilizing HPC for my future research. As long as you have aspirations to conduct research that could utilize HPC resources (which, at this point, almost all fields of research do) and a good plan as to how you will train yourself to use such resources, you will find a great home within this program. The benefits of the program simply are too great not to give yourself a chance.

Benjamin Robert Galloway, Sandia National Laboratories (brgallo@sandia.gov)

Years at SNL: 2018-Present ✦ **Degree:** PhD, Physics ✦ **SSGF:** 2012-2016, University of Colorado, Boulder

As a laser scientist contributing to high energy density physics research at Sandia National Laboratories' Pulsed Power Sciences Center, I am surrounded by unparalleled expertise and awe-inspiring capability. Sandia's Z facility performs a plethora of (literally) ground-shaking experiments in the name of national nuclear security. The Z machine does a lot of heavy lifting to create exotic states of matter, and scientists such as me work to ensure the experiments can be diagnosed to produce accurate physics interpretations. Substantial investments have gone into making the Z facility what it is today, and the number of world experts working together to perform frontier science at Z truly is stunning. I consider myself very fortunate to be part of the action.

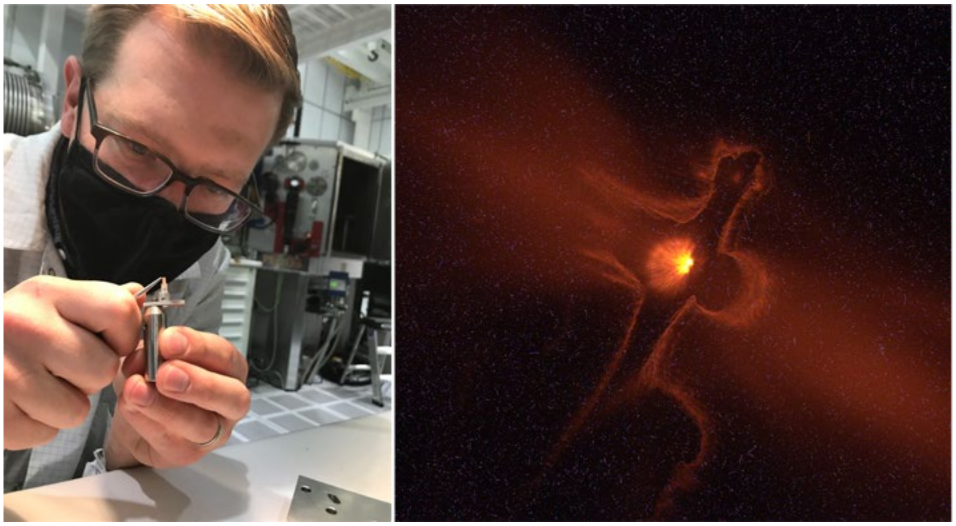


Figure 1. (Left) Benjamin Galloway prepares a foil target for a Z-Petawatt laser experiment. (Right) Side-on Schlieren image of the foil target, captured nanoseconds after the arrival of the Z Petawatt pulse.

In 2018, I joined the team at the Z-Backlighter laser facility where two kilojoule class lasers are maintained to support experimental objectives on the Z machine. One of my primary responsibilities is to act as one of only two operators of the Z-Petawatt laser. This two-person staffing is incredibly lean when compared to other kilojoule/petawatt class laser facilities, allowing me to become intricately familiar with the laser's many subsystems. Our efforts in recent years have expanded the capability of Z-Petawatt for applications in X-ray radiography, particle acceleration, and diagnostic capability development. My role in the Z-Backlighter group is rather unique: not only do I work at the front end of Z-Petawatt to deliver laser light toward end stations, but I also play a large part in the design, setup, execution, and analysis of application experiments at the target chambers (Figure 1). It is quite rare for an individual to routinely work at both ends of such a laser system or to have broad discretion and plentiful beam time to pursue mission-relevant experiments.

"As my career progresses, I will never forget the extraordinary support I've received along the way. I am incredibly grateful to the SSGF program for opening doors for me, and I hope to return the favor through outreach and advocacy for the DOE/NNSA academic programs—programs whose value cannot be understated."

An unusual aspect of my professional career is that Sandia recruited me to the senior staff level directly out of graduate school, bypassing the traditional start in a postdoctoral position. I primarily attribute this to very fortunate timing and having made phenomenal connections through the Stewardship Science Graduate Fellowship (SSGF) program. Whereas the benefits of SSGF are numerous, the networking opportunities enabled by the annual program reviews and laboratory practicum were priceless. During my final year in the Kapteyn-Murnane group at the University of Colorado at Boulder, I barely had given thought to job applications before I was contacted by John Porter, my current manager, and was invited to apply for a timely staff opening. John had found me through SSGF, and as I become more engaged in Sandia's recruitment activities, I similarly find the Department of Energy/National Nuclear Security Administration's (DOE/NNSA) academic programs to be ideal pools to search for talent.

Another benefit stemming from my SSGF experience relates to my 2014 practicum at Lawrence Livermore National Laboratory. There, I participated in a laser wakefield acceleration campaign that inspired me to pursue the same laser application using Z-Petawatt. By securing funding through Sandia's Laboratory Directed Research and Development (LDRD) program, my team now is developing the laser wakefield acceleration platform for novel X-ray diagnostic capabilities on the Z machine. As an early career scientist, the LDRD program is one of my favorite aspects of the national laboratories, because it provides a clearly defined, formal avenue for young scientists to take on increased responsibilities and leadership roles.

As my career progresses, I will never forget the extraordinary support I've received along the way. I am incredibly grateful to the SSGF program for opening doors for me, and I hope to return the favor through outreach and advocacy for the DOE/NNSA academic programs—programs whose value cannot be understated.

Drew Morrill (drewmorrill@colorado.edu)

Degree in Progress: PhD, Physics, University of Colorado, Boulder ✦ **Advisor:** Dr. Margaret Murnane and Henry Kapteyn ✦ **SSGF:** 2018-Present

Research Topic

Ultrafast Lasers for High Harmonic Generation

Research Responsibilities

I am a member of a team of researchers at JILA, a research institute located at the University of Colorado in Boulder. We are developing and building a tabletop-scale laser system that will be used to generate coherent soft X-ray light. The laser system we are building has no blueprints. As a result, our research is highly collaborative, and responsibilities change as our research progresses. We work to stay on top of the latest advances in laser physics and to test new ideas when they might help us reach our goals. For instance, over the past 18 months, we worked closely with the National Institute of Standards and Technology (NIST) Boulder to build an all-fiber, front-end laser that has offered exceptional stability and has allowed us to focus our attention on downstream aspects of the laser system.

Benefits of SSGF

Competitive graduate fellowships like the Stewardship Science Graduate Fellowship (SSGF) seek to cultivate the next generation of leaders in science. Whereas a typical PhD in Physics allows ample time to dive deeply into one specific area of knowledge, it can be difficult to find the time to develop a broader perspective on the role of science in society. Years from now, if any of us find ourselves tasked with guiding the mission of federally-funded science, I think that perspective gained over the course of this fellowship will be invaluable – not so that we can maintain the status quo, but so that we can improve and even reinvent the mission to meet new challenges. Lastly, getting to know the other fellows has given me confidence that the next generation of leaders in science will take seriously the societal implications of their work and that they genuinely wish to apply their talents to the greater good.

What Students Considering SSGF Should Know

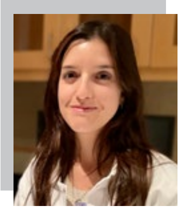
Firstly, bringing your own funding in graduate school might allow you to work with the advisor or group of your choosing. Finding the right advisor may be the most significant factor in the quality of your experience in graduate school. Secondly, the needs of the Department of Energy/National Nuclear Security Administration (DOE/NNSA) research complex are diverse and evolving, so don't be discouraged from applying if you don't think your work aligns perfectly with the mission of stockpile stewardship.

Olivia Pardo (opardo@caltech.edu)

Degree in Progress: PhD, Geophysics, California Institute of Technology ✦ **Advisor:** Dr. Jennifer Jackson ✦ **SSGF:** 2018-Present

Research Topic

Planetary Materials under Extreme Conditions



Research Responsibilities

My research focuses on conducting experiments with planetary materials in order to characterize their structural, vibrational, and electronic properties under conditions relevant to planetary environments. My work involves multi-technique experimental investigations of hydrous, iron-bearing sulfates and informs our understanding of these species' role in localized sulfur-rich environments within the Earth and on icy satellites' surfaces to deep interiors. I use high-pressure devices (diamond anvil cells), coupled with laser heating and cryogenic cooling systems, to achieve the pressures and temperatures of deep planetary interiors. We design experiments and probe these samples with X-ray diffraction, infrared spectroscopy, and nuclear resonant scattering techniques at synchrotron light sources at Department of Energy/National Nuclear Security Administration (DOE/NNSA) laboratories around the country. These techniques are readily transferable to other fields of research studied at the national laboratories; because of this I was able to learn new, high-pressure methods through the fellowship program. During the Stewardship Science Graduate Fellowship (SSGF) practicum, I was able to work with the High Pressure Physics Group at Lawrence Livermore National Laboratory (LLNL) to learn and apply a new dynamic compression technique unavailable at my home institution. Through this practicum, I gained invaluable experience implementing these dynamic compression techniques in the diamond anvil cell and working closely with field-leading scientists at LLNL. I continue to collaborate with my practicum mentors on projects that, while not necessarily in planetary science, utilize the same tools and processes that I have developed as part of my PhD.

Having never toured a national laboratory prior to being an SSGF fellow, my time at LLNL and my experience as a member of the SSGF community were invaluable and have heavily influenced my post-graduation career possibilities. The SSGF program enabled me to feel financially secure in my PhD and helped me gain a community of peers that I would not have been able to explore without the SSGF program. To any student considering the SSGF, the DOE/NNSA laboratories available to you support an incredible variety of research projects with which, you may not realize, your research can be integrated and extended. The support from the fellowship is unmatched, and the conferences, site visits, and practicum opportunities and experiences are uniquely beneficial as you progress in your PhD.

Dane M. Sterbentz, Lawrence Livermore National Laboratory (sterbentz2@llnl.gov)

Years at LLNL: 2021-Present ✦ **Degree:** PhD, Mechanical and Aerospace Engineering, University of California, Davis
✦ Advisor: Dr. Jean-Pierre Delplanque ✦ **LRGF:** 2019-2021

The Laboratory Residency Graduate Fellowship (LRGF) provided me with both the resources and financial support that I needed to focus full time on my PhD research. One of my favorite aspects of the LRGF was the on-site national laboratory residencies which allowed me to collaborate closely with world-class researchers at Lawrence Livermore National Laboratory (LLNL). During these residencies, LLNL staff scientists Dr. Jonathan Belof and Dr. Philip Myint provided me with insightful research guidance and constructive mentoring. These residencies allowed me access to LLNL computing resources and software that were essential for completing my PhD research. Through these on-site laboratory residencies at LLNL, I was able to gain a greater appreciation for the importance and diverse scope of research conducted at a national laboratory. Another of my favorite aspects of the LRGF was attending the annual Stewardship Science Graduate Fellowship (SSGF)/LRGF Program Review. These program reviews allowed me to meet and network with other SSGF/LRGF students as well as national laboratory researchers from across the country. These types of events oftentimes plant the seeds for future collaborations, as well as lifelong friendships, and were a very valuable experience. Through the many exciting research and networking opportunities and the ability to work with some of the top experts in the field of high energy density physics through on-site residencies, this fellowship has convinced me that a national laboratory is one of the best possible places to start a career for a PhD graduate and steered me to my current position as a postdoctoral researcher at LLNL.

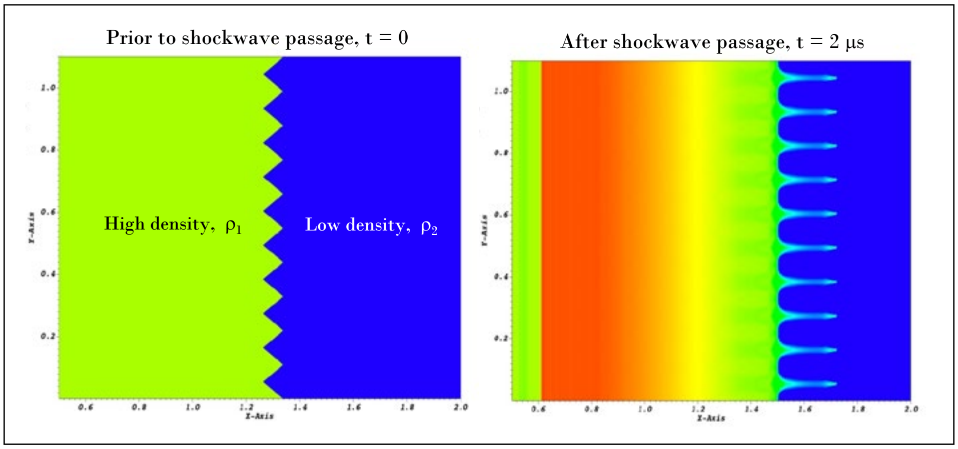


Figure 1. Hydrodynamic simulation of the Richtmyer-Meshkov instability (RMI). The plot on the left shows the initial interface between two materials of different densities prior to shockwave passage. The plot on the right shows the unstable RMI spike growth that occurs after shockwave passage. Photo Credit: D. Sterbentz , LLNL

> *"Another of my favorite aspects of the LRGF was attending the annual Stewardship Science Graduate Fellowship (SSGF)/LRGF Program Review. These program reviews allowed me to meet and network with other SSGF/LRGF students as well as national laboratory researchers from across the country. These types of events oftentimes plant the seeds for future collaborations, as well as lifelong friendships, and were a very valuable experience."*

My postdoctoral research project involves the suppression and control of perturbation growth from the Richtmyer-Meshkov instability (RMI) in shock-compressed materials. RMI is a phenomenon that occurs at the interface of two substances of different densities due to an impulsive acceleration, such as a shock wave passing through this interface. Under these conditions, perturbations at the interface begin to grow due to the RMI, which leads to the propagation of jets or spikes of one substance into the other (see Figure). One major challenge encountered in inertial confinement fusion applications, which generally use high-pressure shock waves to compress a fuel target, is asymmetry during the implosion process due to RMI that reduces the energy yield. The suppression of perturbation growth caused by RMI is an important, yet challenging, goal. My postdoctoral research uses hydrodynamic simulations of impactor shock-wave experiments and methods based in design optimization to suppress RMI growth by altering the geometry and other properties of a shocked material target. Our results show that a secondary instability can be created intentionally to counteract RMI growth at a perturbed interface.

I conduct much of my postdoctoral research in collaboration with experimentalists who develop shock-wave compression experiments at LLNL's High Explosives Application Facility (HEAF), as well as at the Dynamic Compression Sector (DCS) beamline at Argonne National Laboratory. Our simulations have been helping to inform the design of new shock-wave compression experiments at both HEAF and DCS for studying RMI. I also have been continuing work (started during my PhD) on studying phase transition kinetics occurring under the extreme pressures encountered in dynamic-compression experiments which use shock or ramp waves to compress a material sample. For the case of solidification, these experiments often compress the liquid sample so rapidly that the material becomes deeply undercooled past the phase boundary before solidification actually occurs. The main objective of this work is to better understand how the nonequilibrium phase transition kinetics affect the conditions at which the phase transition occurs, which can help us to deconvolve where the true equilibrium phase boundaries lie for materials at high pressures.

Patricia Cho (patricia.cho@utexas.edu)

Degree in Progress: PhD, Astronomy, University of Texas at Austin ✦ **Advisor:** Dr. Don Winget ✦ **LRGF:** 2020-Present

Research Topic

Laboratory Astrophysics

Research Responsibilities

My research responsibilities center around fielding experiments on the Z machine designed to answer questions related to accreting black hole systems. The work ranges from identifying specific research goals, designing and fielding the experiments, data processing, and running simulations in service of the data analysis.

Benefits of LRGF

The Laboratory Residency Graduate Fellowship (LRGF) program has facilitated my integration into Sandia National Laboratories (Sandia) in a way that enables me to pursue my scientific interests and research goals at a level that would otherwise be impossible. The Z machine allow us to access regimes which are otherwise terrestrially unobtainable and provides a singular platform to study photoionized plasmas. Interaction with Sandia scientists as well as the larger network of astrophysicists at other national laboratories as well as universities provides me with unique and valuable exposure to a much wider cross-section of the scientific community.

National Laboratory Experience

Black holes remain some of the most enigmatic and powerful astrophysical objects that we know of. Our understanding of these objects is facilitated by ever improving instrumentation aboard space-based satellite observatories and by simulation codes like XSTAR, which is used to model accreting black hole systems. The simulations involve a vastly complicated and interconnected network involving, among other things, atomic structure calculations, relativistic effects from the extreme gravitational field induced by the singularity, and an account of the various components of the system including the processes involved in the accretion disk. The temperatures and densities of the plasmas found in the accretion disks around black holes are already challenging for terrestrial laboratories to reach. The fact that these plasmas are photoionized requires an extremely powerful X-ray source and makes replicating the conditions near impossible. Our understanding of these systems is limited in part by our ability to study the detailed microphysics at the specific conditions of these accreting plasmas.

As a graduate student in an astronomy program, I hadn't considered and wasn't aware of the opportunities at the national labs. My serendipitous introduction to laboratory astrophysics research being enabled by high energy density facilities like the Z machine started with my graduate advisors.

I have been fortunate to remain in long -term residence at Sandia and to field experiments on the Z machine related to outstanding questions about these accreting black hole systems. The ability to successfully field experiments on a facility like Z requires dedicated and sustained effort involving the expertise of experimentalists, theorists, engineers, and technicians.

William Riedel (wriedel@stanford.edu)

Degree in Progress: PhD, Mechanical Engineering, Stanford University ✦ **Advisor:** Dr. Mark Cappelli ✦ **LRGF:** 2018-Present

Research Topic

Kinetic Effects in Converging, Fully-ionized Plasma Jets

Research Responsibilities

I study kinetic behavior in plasmas at extreme temperatures and densities relevant to inertial confinement fusion. Plasmas in this regime typically are modeled using the fluid approximation, which assumes that the collisional mean-free-path of an ion is much smaller than the scale length of interest. But this assumption often is violated, and certain behaviors (e.g. interpenetration, diffusive mixing, beam-beam fusion) can occur that cannot be captured with a fluid model.

Primarily, I conduct kinetic-ion simulations of a novel laser-fusion target that allows for wide control over the collisionality of the system. These experiments generate spherically converging plasma jets that travel inward either through vacuum or in a low-density background gas. In vacuum, these jets interpenetrate deeply at the target center, altering the structure of the stagnation process and the densities and temperatures achieved. In the presence of a background gas, we have shown the potential for significant mix of the shell plasma into the gas through the formation of a weakly collisional electrostatic shock. This effect is detectable through fusion neutron yield scaling vs. gas pressure. Simulation predictions show excellent agreement with experimental data recorded at the OMEGA laser facility, suggesting that 1D kinetic mechanisms are sufficient to explain the results without considering other possible sources of mix.

Benefits of LRGF

The support provided by Laboratory Residency Graduate Fellowship (LRGF) program has given me the ability to focus full-time on my research and the freedom to choose my research direction. I have been able to connect and collaborate with researchers at the national laboratories (in my case, Lawrence Livermore National Laboratory (LLNL)) who have contributed greatly to my academic and professional development and have been a resource to turn to when I am looking for advice. I also have been able to take advantage of LLNL's world-class computing clusters and to get involved with experimental campaigns at both the OMEGA and National Ignition Facility (NIF) laser facilities.

Through the LRGF/Stewardship Science Graduate Fellowship (SSGF) network and annual program reviews, I have been exposed to a broad sampling of research areas and career paths and have gotten the chance to spend time with peers from across the country.

National Laboratory Experience

The LRGF program particularly emphasizes and encourages stronger collaboration with researchers at the national laboratories. Because of this, you will often gain another mentor who has a vested interest in your growth. That is a valuable benefit!

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.

— Overview, page 5

User Facilities

> *New General Users are, once again, encouraged to submit proposals for experimental time. 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 https://dcs-aps.wsu.edu/proposal-submission for information regarding GU proposal submission.*
>
> **— Dynamic Compression Sector**

> *In addition to various experimental efforts, capability developments, and strong user support, HPCAT is dedicated to continuing vital student engagement and training. Due to various restrictions and limitations to onsite user visits since March of 2020, the hosting of offsite students has been hampered severely. However, as HPCAT continues to push towards broader work resumption and user visits, a number of onsite students recently have been hosted.*
>
> **— High Pressure Collaborative Access Team**

Dynamic Compression Sector: Return to Onsite User Operations

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

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/National Nuclear Security Administration (DOE/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.

The DCS's uniqueness and extreme versatility arise from the combination of different dynamic compression drivers, a broad range of X-ray beam characteristics (energies and pulse separations), and the ability to obtain *in-situ*, real-time measurements at continuum-to-atomistic length scales. Using the different experimental stations (Impact Facilities, Laser-Shock, and Special Purpose), time-resolved X-ray (diffraction, phase contrast imaging, scattering, and absorption spectroscopy) and continuum (laser interferometry) measurements are available for a wide range of user experiments. Past studies have successfully addressed long-standing, scientific challenges. Visit https://dcs-aps.wsu.edu for details regarding DCS capabilities, publications (2016-present), and guidance for user experiments.

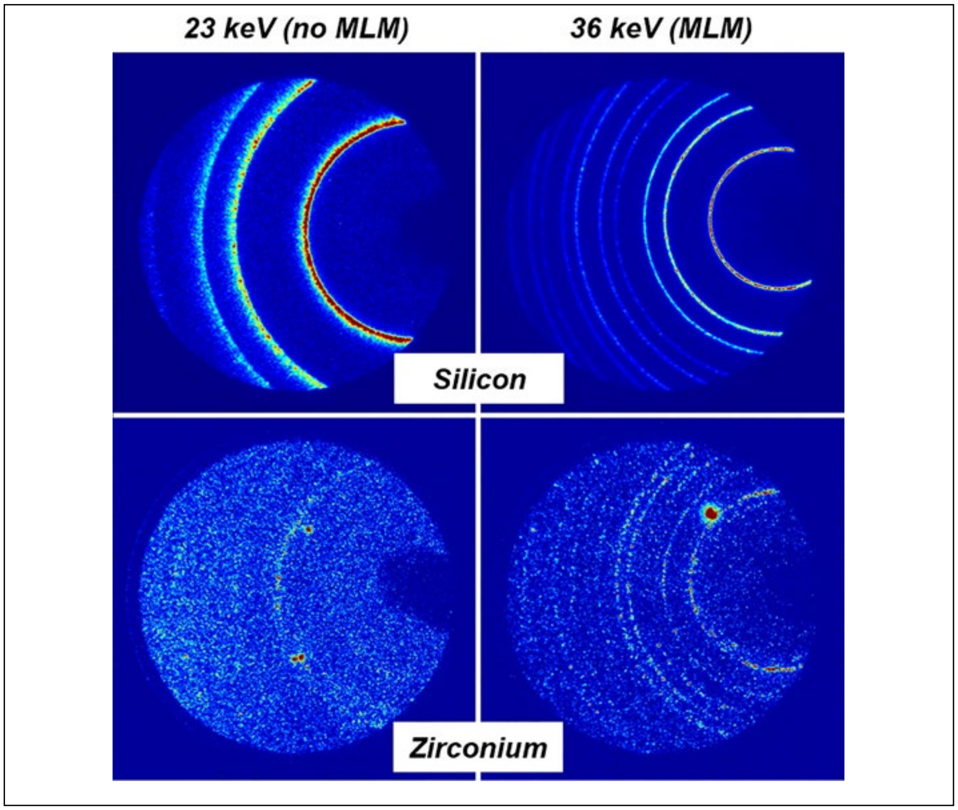


Figure 1. High energy X-ray diffraction measurements at 36 keV provide a first-in-class capability for dynamic compression experiments.

Recent Enhancements

New capabilities were developed at the DCS over the past year, and the same are summarized briefly. Development of a multilayer monochromator (MLM) system to isolate a single, high-energy harmonic from the undulator spectrum—an important need identified by the DCS user community—was undertaken. Experiments in the Impact Facilities demonstrated the ability to isolate X-rays at 36 keV producing diffraction patterns with excellent signal-to-noise (Figure 1). Without MLMs, isolating X-ray energies greater than 24 keV for diffraction measurements was not possible. MLMs will be installed in each station during Run 2022-1 to provide spectral filtering and to enable clean, hard X-ray measurements—a significant advancement required to leverage the X-ray beam enhancements in the APS Upgrade. For laser shock experiments, two new capabilities will be available: 1) finer pulse energy tuning for users by energy adjustment through early stages of the laser system and 2) the second leg of the line-VISAR for high spatial resolution measurements.

Return to Onsite Experiments

The COVID-19 pandemic and the associated restrictions to onsite experimental work resulted in significant disruptions to the DCS operations. The DCS staff developed appropriate operational and experimental procedures for safely conducting user experiments remotely in the Laser Shock and Impact Facilities with extremely limited DCS staff allowed onsite. The remote experiments were conducted with experienced Collaborative Access Team (CAT) members, because onsite training for new users is required. By Run 2020-3 the DCS staff could support a full schedule of user experiments, and in Run 2021-1, the remote user operations were expanded to include experienced General Users. Overall, the DCS staff performed over 1000 experiments remotely – a remarkable achievement. However, remote experiments at the DCS are not sustainable over the long run. Also, certain experiments cannot be carried out remotely and require the onsite presence of users.

For Run 2021-3, the DCS worked with the Advanced Photon Source to safely return to onsite operations, and time was allocated for new General Users who had previously submitted proposals following the Argonne site access requirements. New General Users are, once again, encouraged to submit proposals for experimental time. 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 https://dcs-aps.wsu.edu/proposal-submission/ for information regarding GU proposal submission.

User Facilities: High Pressure Collaborative Access Team

Advanced Photon Source, Argonne National Laboratory ✦ Author: Dr. Nenad Velisavljevic (HPCAT-Director@anl.gov)

The High-Pressure Collaborative Access Team (HPCAT) is a synchrotron-based high-pressure research facility dedicated to providing cutting-edge experimental capabilities that enable National Nuclear Security Administration (NNSA) laboratories—Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Sandia National Laboratory (SNL)—NNSA Stewardship Science Academic Programs (SSAP), as well as the broader scientific community, to investigate matter at pressure-temperature (P-T) extremes using X-rays. In addition to supporting a diverse user community, HPCAT also performs research and development of synchrotron X-ray techniques for application to studying materials under extreme P-T conditions; development of new devices and platforms for generating high P-T conditions; and the training of students and postdoctoral researchers in support of providing the next-generation workforce at the national laboratories.

The HPCAT facility is comprised of four simultaneously operational X-ray end-stations and various supporting sample preparation laboratory space. The end-stations offer a suite of experimental X-ray probes that span spectroscopy, diffraction, microscopy, radiography, and tomography. The end-stations are setup to accommodate a variety of diamond anvil cells (DAC) and Paris-Edinburg (PE) cell assemblies and are coupled with white beam, pink beam, and a monochromatic X-ray beam for *in situ* measurements at high pressures up to 500 GPa and temperatures of more than 4000 K. The experimental platforms enable the determination of strength, volume, structure, and bonding at extreme P-T conditions and constitute key data that are used to validate theoretical models and support various NNSA mission-focused projects. The details and scope of the available techniques are communicated to our users via the HPCAT website https://hpcat.aps.anl.gov/. HPCAT also has contributed to the design and development of new capabilities and has supported partner users toward achieving greater pressures, temperatures, and strain rate conditions. In one recent study, using a DAC and *in situ* X-ray measurements, our partner user group from LLNL was able to determine the pressure-volume (P-V)compression curve of silver up to 416 GPa (Figure 1(a)) which is hundreds of GPa greater than previously reported studies[1]. Likewise, ongoing developments with PE cell capability (Figure 1(b)), have extended the achievable conditions to megabar pressures[2,3]. The PE press provides a larger sample volume for investigating amorphous materials and performing various radiography and tomography measurements. The emergence of new experimental techniques and improved X-ray measurements also has necessitated the development of next-generation experimental data analysis tools. Using various X-ray and high pressure platforms at HPCAT and other light sources and with complementary efforts at home institution, our partner group from LANL's Applied Computer Science and Shock & Detonation Physics Groups recently developed Cinema:Snap[4], a software tool designed for the management and visualization of very large high-pressure X-ray diffraction datasets (Figure 1(c)). These software platforms allow users to perform faster data analysis and make real time decisions during an experiment to improve the quality of experimental results and maximize the use of scarce experimental facility time.

In addition to various experimental efforts, capability developments, and strong user support, HPCAT is dedicated to continuing

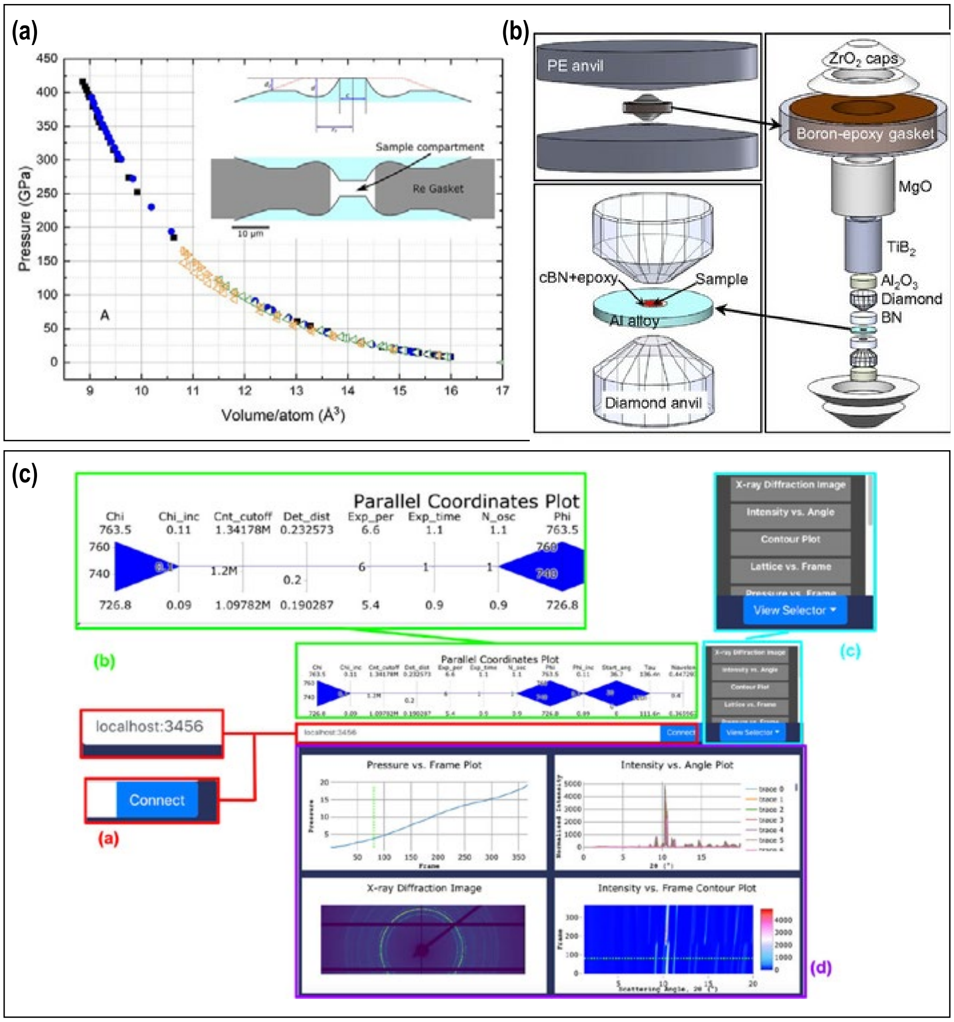


Figure 1. (a) Pressure-Volume data compiled from a diffraction study on silver to pressures above 400 GPa by HPCAT partner user group from LLNL showing the stability of the fcc (cubic) phase to highest pressures[1]. (b) Double stage assembly for achieving 100 GPa pressures with a PE cell[2,3]. Newly developed software by HPCAT partner user group from LANL provides users at HPCAT and other light sources with faster data analysis and improvements in real time decisions toward higher quality experimental measurements[4].

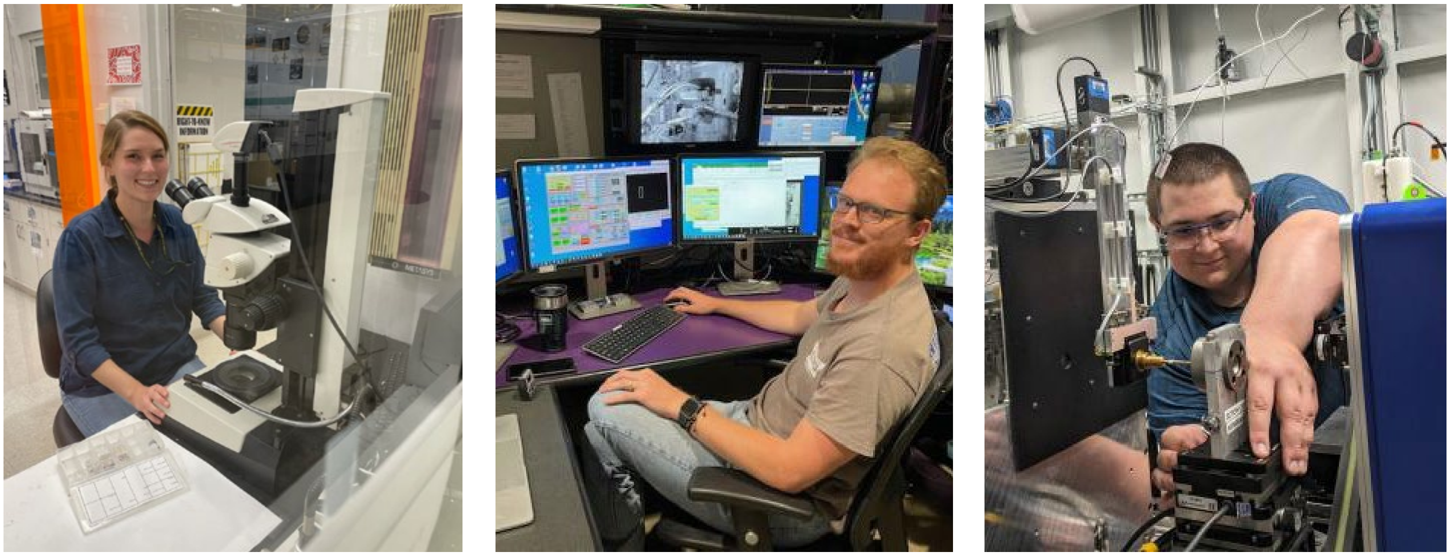


Figure 2. Students visiting and training with HPCAT staff (L to R): Megan Mouser, academic user group member out of University of Tennessee, Knoxville; Seth Iwan from NNSA-SSAP partner Professor Y. Vohra's University of Alabama Birmingham group; and NNSA Stewardship Science Graduate Fellow, John Copley from Professor Tom Duffy's Princeton University group.

vital student engagement and training. Due to various restrictions and limitations to onsite user visits since March of 2020, the hosting of offsite students has been hampered severely. However, as HPCAT continues to push towards broader work resumption and user visits, a number of onsite students have been hosted recently. Graduate students: Seth Iwan from NNSA-SSAP partner, Professor Yogesh Vohra's University of Alabama Birmingham group; Megan Mouser from one of our academic user group members out of the University of Tennessee, Knoxville; and NNSA Stewardship Science Graduate Fellow (DOE NNSA SSGF https://www.krellinst.org/ssgf/), John Copley from Professor Tom Duffy's Princeton University group, all have spent significant time at HPCAT working on new technique development, engaging with NNSA partners, and learning various aspects of X-ray and high pressure measurements (Figure 2).

References

[1] E.F. O'Bannon, M.J. Lipp, J.S. Smith, Y. Meng, P. Söderlind, D. Young, and Z. Jenei, The ultrahigh pressure stability of silver: An experimental and theoretical study, J. Appl. Phys., 129, 125901 (2021). https://doi.org/10.1063/5.0045374

[2] Y. Kono, Y. Shibazaki, C. Kenney-Benson, Y. Wang, and G. Shen, Pressure-induced structural change in MgSiO3 glass at pressures near Earth's core-mantle boundary, PNAS, 115, 1742 (2018). https://doi.org/10.1073/pnas.1716748115

[3] Y. Shu, Y. Kono, I. Ohira, R. Hrubiak, C. Kenney-Benson, M. Somayazulu, N. Velisavljevic, and Guoyin Shen, Structural changes in liquid lithium under high-pressure, J. Phys. Chem. B 2020, 124, 33 (2020) https://doi.org/10.1021/acs.jpcb.0c05324

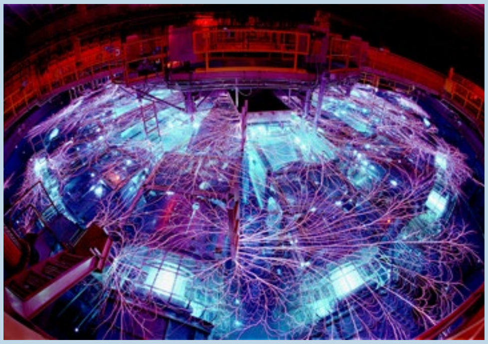
[4] C.M. Biwer, A. Quan, L.Q. Huston, B.T. Sturtevant, and C.M. Sweeney, Cinema:Snap: Real-time tools for analysis of dynamic diamond anvil cell experiment data, Review of Scientific Instruments 92, 103901 (2021). https://doi.org/10.1063/5.0057878

User Facility Summaries

Dynamic Integrated Compression Experimental Facility

The Dynamic Integrated Compression Experimental (DICE) facility at Sandia National Laboratories provides multiple platforms for material property study utilizing both gun launched projectiles and pulsed power accelerators 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 of sample response under different loading conditions. Primary diagnostics include laser-based velocimetry (PDV, VISAR) and high-speed videography. For more information visit http:// www.sandia.gov/Pulsed-Power/research_facilities/index.html. Interested users may contact Scott Alexander (calexa@sandia.gov) for more information.

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 https://www.sandia.gov/pulsed-power/ or contact Marcus Knudson, mdknuds@sandia.gov.

Shock Thermodynamic Applied Research

The Shock Thermodynamics 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. STAR houses a collection of five laboratory test launchers (guns) used for dynamic material property and ballistic impact studies. It is unique in the world in that the collection of launchers can achieve a wide range of sample pressure (bars to multi-Mbar) for material property study. The facility is also equipped to perform ballistics studies with a diverse range of projectile shapes, sizes, and materials. Primary diagnostics include laser-based velocimetry (PDV, VISAR), high-speed videography, and flash x-radiography. For more information visit http:// www.sandia.gov/Pulsed-Power/research_facilities/index.html. Interested users may contact Scott Alexander (calexa@sandia.gov) for more information.

Omega Laser Facility

The Omega Laser Facility at the University of Rochester's Laboratory for Laser Energetics (LLE) includes the 60-beam OMEGA and the 4-beam high-energy, high-intensity OMEGA EP Laser Systems. The OMEGA EP short pulse beam (up to 2) or the tunable-wavelength long-pulse beam can also be transported to the OMEGA chamber for joint operations. The facilities have been adapted to operate experiments for remote users. The two lasers share over 100 facility-supported diagnostics and perform over 2000 highly diagnosed experimensts annually. LLE staff work closely with the User Community via the Omega Laser Facility Users Group (OLUG) to improve and add new capabilities every year. Nearly one-third of the experiments at the Omega Laser Facility support basic high energy density science. Three programs provide general user access with beam time granted through a peer-reviewed proposal process (National Laser Users' Facility and Laboratory Basic Science funded by NNSA, and LaserNetUS funded by DOE's Office of Fusion Energy Sciences). Application details are available on the LLE website for the NLUF and LBS programs, on the LaserNetUS website for additional beamtime on OMEGA EP. For more information, visit https://www.lle.rochester.edu/ or contact Dr. Mingsheng Wei, NLUF Manager, 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 high energy, synchrotron x-ray capabilities (36 keV) 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 (APS), 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 operational schedule at HPCAT, along with the host APS facility, is divided into three cycles per year – the calendar time-frame of each cycle and any updates can be found on the APS home website. For those interested in performing work at HPCAT the experimental time can be obtained via the General User Proposal (GUP) peer review system or internal partner time allocation request. If interested in GUP additional information can be found at https://www.aps.anl.gov/Users-Information/About-Proposals/Proposal-Types/General-User-Proposals. For partners (including LLNL/ LANL/SNL and NNSA-SSAA PIs) please email HPCAT-Director@anl.gov to discuss dedicated beamtime allocation, experimental scope/requirements, 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, neutron radiography, and radiography nuclear physics, and the Weapons Neutron Research Facility for nuclear physics, neutron radiography, and electronics testing. 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, neutron irradiation for industrial application, 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 main 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.

FY 2022 Funded 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
Chikang Li
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 Chicago
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Aqueous-Phase Isotope Harvesting to Manufacture Radioactive Targets for Neutron-Reaction Studies

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A Novel Technique for the Production of Robust Actinide Targets

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Seeing Through the Fission: Multi-Modal Analysis of Actinides and Noble Gas Isotopes in Geological Samples

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Yogendra Gupta
Dynamic Compression of Materials: Multiscale Measurements and Analysis

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Argonne National Laboratory

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Resonant Excitation and Multistage Amplification of Electron Plasma Waves in High Energy Density Plasmas

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X-Ray Spectroscopic Studies of Radiative Collapse in X-Pinch Plasmas

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Johan Frenje
Development of New Advance+d X-ray and ▯-ray Diagnostics for Inertial-Confinement-Fusion and Discovery-Science Programs at OMEGA and the NIF

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Derek Schaeffer
Particle Heating by High-Mach-Number Collisionless Shocks in Magnetized Laboratory Plasmas

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Magnetic Reconnection in High-Energy-Density Plasmas

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Pipeline Development of Skilled Workforce in STEM through Advanced Manufacturing (STEAM)

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Successful Training and Effective Pipelines to National Laboratories with STEM Core (STEP2NLs)

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Dr. Jianzhi (James) Li
Consortium of Advanced Additive Manufacturing Research and Education for Energy Related Systems (CA2REERs)

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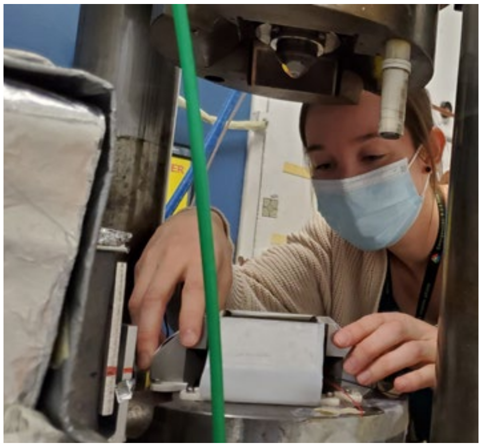
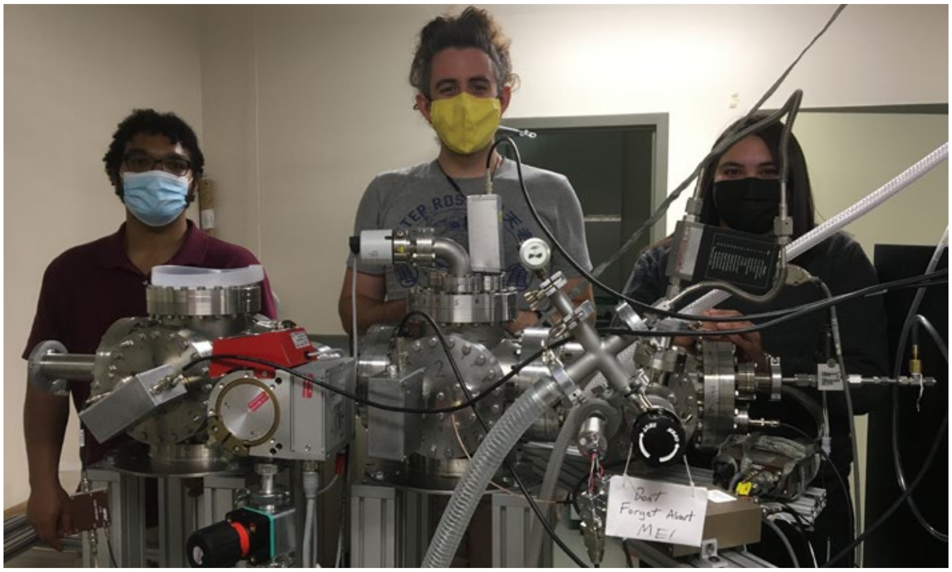
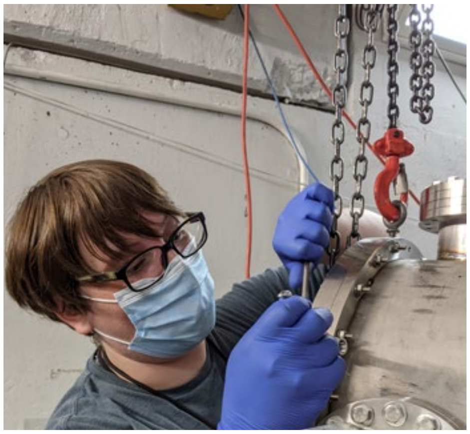
Integrated Additive Manufacturing – Establishing Minority Pathways: Opportunities for Workforce-development in Energy Research and Education (IAM-EMPOWEREd)







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The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) provides up to four years of financial support for students pursuing doctoral degrees in fields that use high-performance computing to solve complex problems in science and engineering.

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A radiation hydrodynamic simulation using a 3-D model of an 80-solar-mass star. Visualization: Joseph A. Insley, Argonne National Laboratory PI: Lars Bildsten, University of California, Santa Barbara

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The Department of Energy National Nuclear Security Administration Laboratory Residency Graduate Fellowship **(DOE NNSA LRGF)** gives students the opportunity to work at DOE NNSA facilities while pursuing degrees in fields relevant to nuclear stockpile stewardship: **engineering and applied sciences, physics, materials, or mathematics and computational science.**

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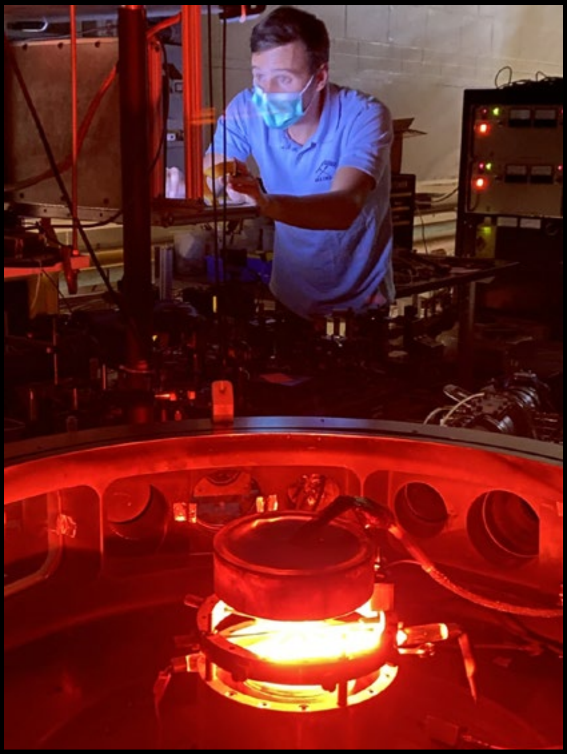

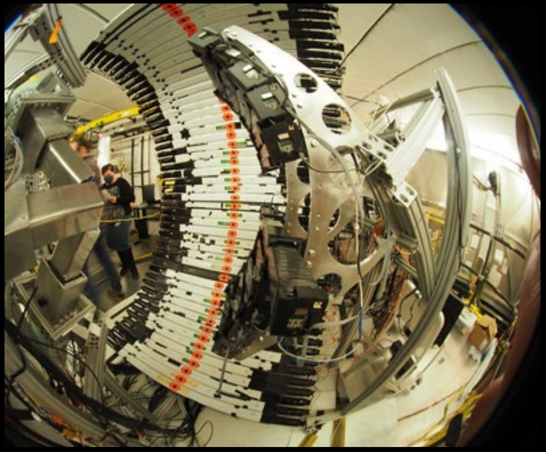

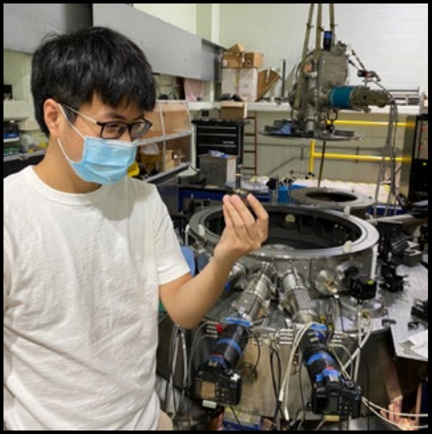

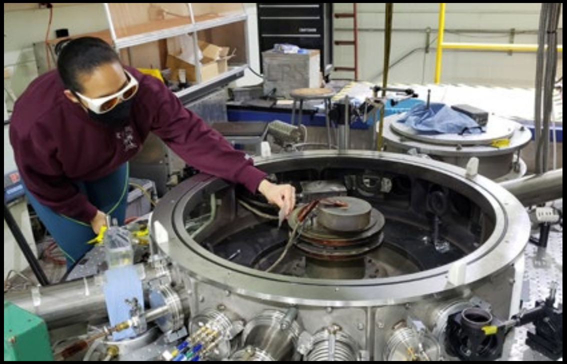

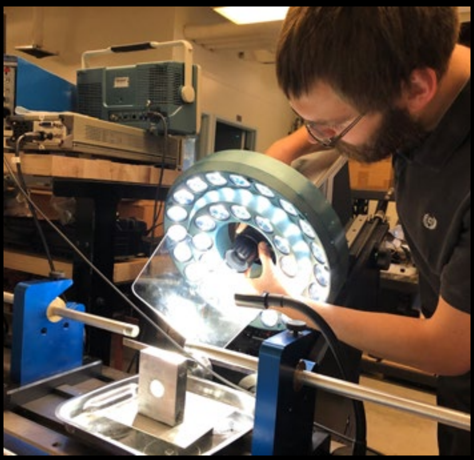

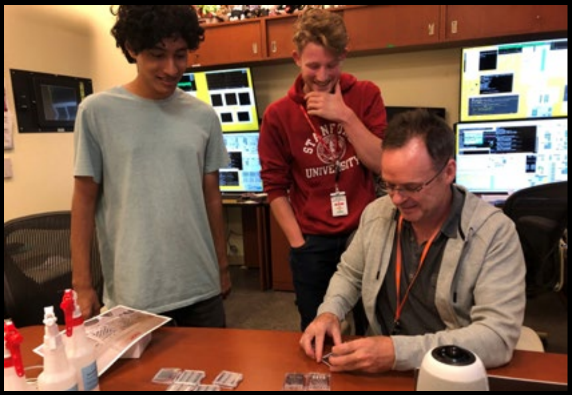
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