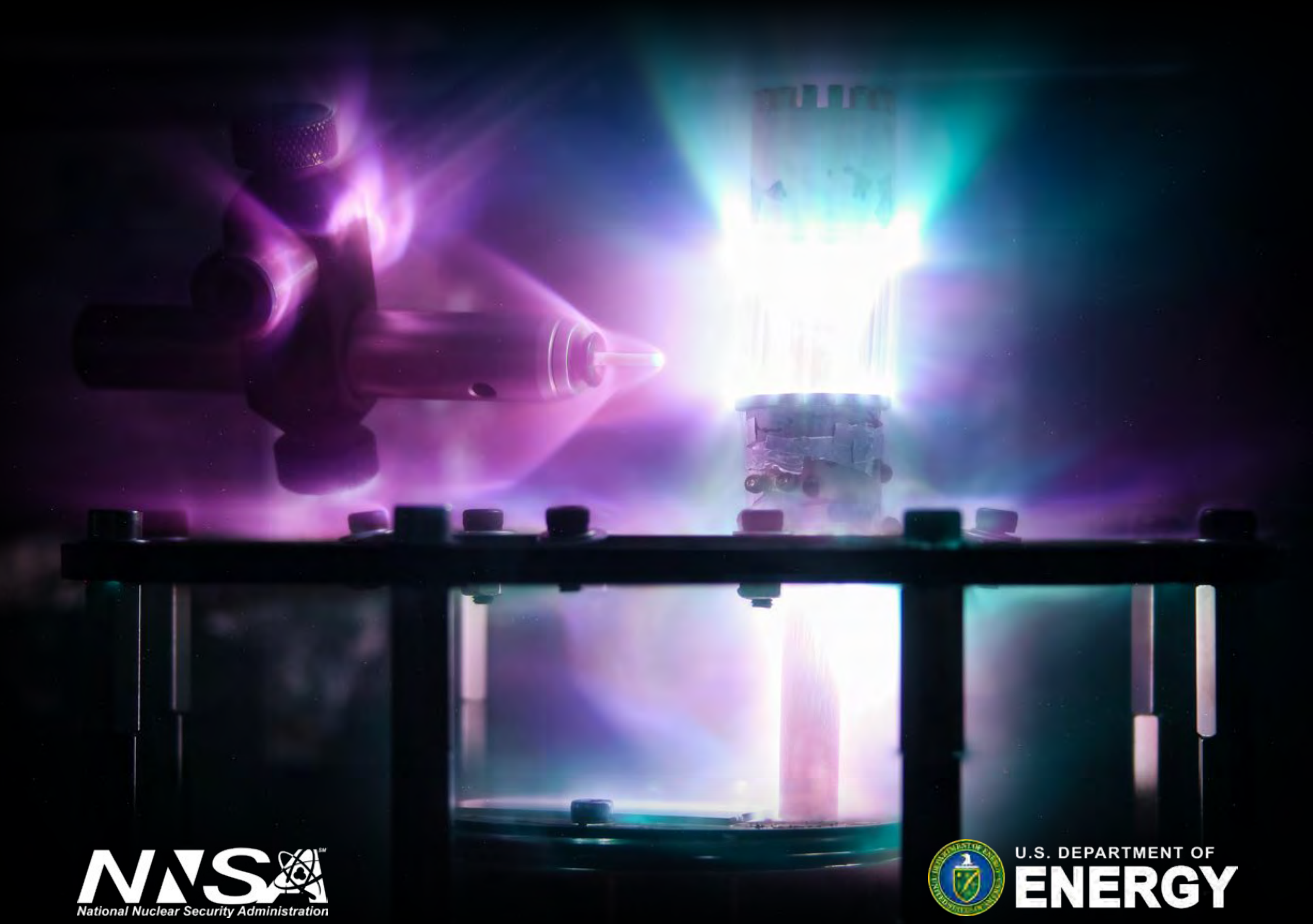
DOE/NA-0139

2023
Academic Programs Annual

NNSA Office of Defense Programs

- Stewardship Science Academic Alliances
- High Energy Density Laboratory Plasmas
- 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

Long exposure photograph of experiment exploring collisionless shocks on MAGPIE.

— Image courtesy of Cornell University

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NNSA National Nuclear Security Administration

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National Nuclear Security Administration

2023 Academic Programs Annual

NNSA Office of Defense Programs

Assistant Deputy Administrator (Acting)
Strategic Partnership Programs

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The Academic Programs Annual is produced by the NNSA Office of Defense Programs. It features select research conducted by the following NNSA-supported research programs: Stewardship Science Academic Alliances, High Energy Density Laboratory Plasmas, Predictive Science Academic Alliance Program, Minority Serving Institutions Partnership Program, and fellowship programs.

Please submit comments to:

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NNSA will recruit, invest in, and nourish a high-performing, diverse, and flexible workforce that can meet the unique policy, technical, and leadership needs of our mission today and well into the future. We champion all aspects of diversity, equity, inclusion, and accessibility so that NNSA and its enterprise benefit from the full range of America's talent. Efforts to minimize personnel attrition are a high priority, as is investing in university programs to support our future workforce.

2022 NNSA Strategic Vision

Welcome from the

Assistant Deputy Administrator (Acting) for Strategic Partnership Programs

What an exciting year it has been for the National Nuclear Security Administration (NNSA). If you are unfamiliar with our mission, we work to ensure that the Nation's stockpile of nuclear weapons remains safe, secure, and effective without performing nuclear testing. This means that we rely on ever-evolving, ground-breaking science, technology, and engineering to accomplish this mission, and we work to support the research of our academic partners in key fields to ensure our continued success and to train and recruit top talent from these academic institutions into the workforce of the NNSA and our national laboratories, plants, and sites.

Although the scientific accomplishments of our programs over this past year were many, one made national news and has great potential for continued, significant advancement in stewarding the Nation's stockpile of nuclear weapons and in advancing the science of fusion energy. If you have not heard, laboratory ignition was achieved at the NNSA's National Ignition Facility (NIF) located at Lawrence Livermore National Laboratory. In the experiment, 2.05 megajoules (MJ) of laser energy were delivered to a target that then output 3.15 MJ of fusion energy. You read that correctly—more energy was output from the experiment than went in. The quest to achieve ignition in a controlled laboratory setting has been seven decades in the making, and this year it was achieved at an NNSA facility! What a great time it is to join our workforce. We conduct ground-breaking science.

The mission of the NNSA is in the interest of national security. The work that we do ensures that the world-at-large remains safe through nuclear deterrence. Nuclear deterrence has been shown to be effective, but it must be strengthened continually by evolving scientific discovery through 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 means you! This is the vital role that the NNSA Academic Programs (AP) serve. The value of the work of the AP to build a safer world is evident in the pages of this Annual. We feature select students pursuing research at our facilities who write in their own words about their experiences with the AP and the opportunities that it has afforded them. We are honored to have all of you as part of our community, and we are especially grateful for our community members who have gone on to careers with the national laboratories, plants, and sites. Many of those community members were part of the team who achieved ignition at the NIF!

To all who are part of our AP community, I wish you a successful year. To everyone else, know that we are always looking for exceptional candidates who want to be part of groundbreaking, world-changing science!

Dr. Njema J. Frazier

Assistant Deputy Administrator (Acting)
Strategic Partnership Programs
National Nuclear Security Administration

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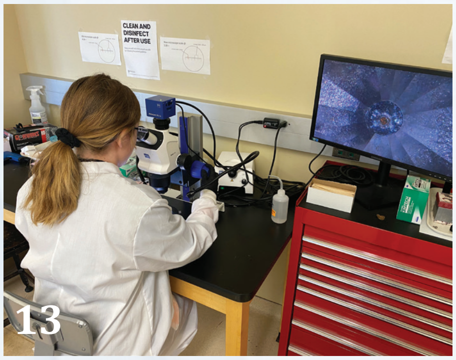

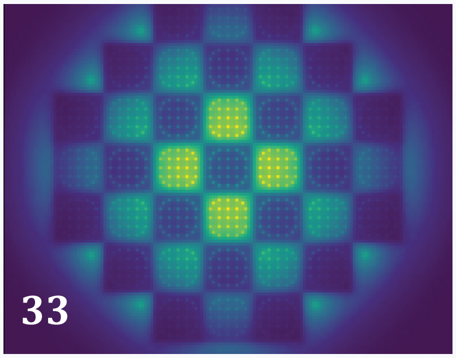
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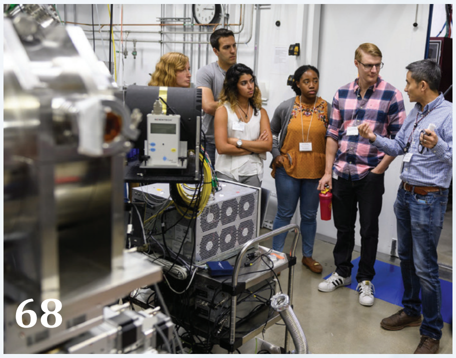
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The Academic Programs enable a robust and diverse research and science, technology, engineering, and mathematics (STEM) educational community through a variety of methods of support.

Overview

Academic Programs

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 Defense Programs (DP) 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.

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 DOE/NNSA missions and to provide direct experiences at the 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 DOE/NNSA mission, and a view to future needs and opportunities of the NSE.

SSGF Fellow Griffin Glenn aligns optics used in an experiment at the Matter in Extreme Conditions endstation at the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory.

The Academic Programs is comprised of the following subprograms:

- Stewardship Science Academic Alliances
- High Energy Density Laboratory Plasmas
- Predictive Science Academic Alliance Program
- Minority Serving Institutions Partnership Program
- Tribal Education 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 properties of materials under extreme conditions and energetic environments; hydrodynamics, instabilities, and hypersonics; low-energy nuclear science; high energy density physics; and radiochemistry. SSAA funding supports research at U.S. universities, training hundreds of 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.

High Energy Density Laboratory Plasmas

High energy density (HED) science is central to many aspects of nuclear weapons and to maintaining a strong HED academic community in this unique field will be critical for the future needs of a modern nuclear stockpile. The High Energy Density Laboratory Plasmas (HEDLP) program 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 individual investigator research grants, centers of excellence, and the Facility Access and Community Development Programs.

Individual Investigator Grants

NNSA's Office of Defense Programs partners with the DOE's Office of Fusion Energy Sciences to issue an annual joint solicitation for high energy density laboratory plasmas (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 HEDLP program 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.

Facility Access and Community Development Programs

The Facility Access Program provides travel support for researchers who have been granted shot time at the Omega Laser Facility. The Omega Laser Facility houses both the OMEGA and OMEGA EP lasers and allows for hands-on research experience to academic and industrial partners. This year, travel support will also be offered to researchers who have been awarded time at NIF and other NNSA facilities. The HEDLP program also provides funding for student travel to attend the High Energy Density Science summer school and various facility workshops.

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 consists of the following types of centers: Multi-disciplinary Simulation Centers (MSCs), Single-Discipline Centers (SDCs), and Focused Investigatory Centers (FICs). MSCs focus on scalable application simulations, targeting large-scale, integrated, multidisciplinary problems, whereas SDCs focus on scalable application simulation for targeting a broad single science or engineering discipline. FICs are tightly focused on a specific research topic of interest to NNSA's mission in either a science/engineering discipline or an exascale-enabling technology.

PSAAP has a long-term goal to cultivate the next generation of scientists and engineers to support the Advanced Simulation and Computing and Stockpile Modernization 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) aim to make the NNSA/DOE workforce diverse, highly skilled, agile, and fully prepared for the future of the DOE/NNSA enterprise. To achieve this vision, MSIPP and TEPP strive to develop a sustainable pipeline that prepares a diverse workforce through partnerships and recruitment programs between MSIs and DOE/NNSA labs, plants, and sites.

MSIPP and TEPP are vital programs within the DOE/NNSA Management and Budget office, under Learning and Career Management. MSIPP and TEPP award grants to MSIs, 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.

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 DOE/NNSA enterprise. To execute this mission, MSIPP and TEPP build and support a network of NSE-ready students through enrichment activities from K–20 to postdoctoral levels. Through university-national lab consortia partnerships, students are exposed to cutting-edge research and activities in their relevant fields.

MSIPP supports all MSIs, including Historically Black Colleges and Universities (HBCUs), Hispanic Serving Institutions (HSIs), and Tribal Colleges and Universities (TCUs) through competitive, consortia-based grant awards with a 3–5-year period of performance. Through the consortia, MSIPP invests in a diverse portfolio including student enrichment programs, curriculum 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. 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 underrepresented colleges and universities.

This alignment is defined by four critical goals:

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

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. CSGF is jointly sponsored with the DOE 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.

Stewardship Science Academic Alliances Program: 20 Years and Counting

by Michael Kreisler, Contractor to the National Nuclear Security Administration Defense Programs

It is hard to believe that it has been 20 years since the start of the Stewardship Science Academic Alliance (SSAA) Program. The SSAA program was initiated to provide funding to universities in areas that other agencies were not supporting and that were important to the nuclear security enterprise. The disciplines include low energy nuclear science, properties of materials under extreme conditions, radiochemistry, and high energy density physics. An overarching goal of the program is to increase the pipeline of scientists interested in careers at the National Nuclear Security Administration (NNSA) national laboratories.

The success of the SSAA program truly has been remarkable. The program has funded research projects in almost all of the States, has produced a large number of scholarly articles, and has supported an enormous number of PhD candidates in their academic careers. Advanced research capabilities were developed at both universities and at laboratories that are now part of the NNSA system.

The program supports individual investigator grants and awards for Centers of Excellence involving many investigators and often multiple institutions. Each project is required to submit an annual research progress report that is reviewed by the NNSA. These reports document the efforts of the academic community to investigate extremely difficult scientific problems.

The NNSA laboratories report that students and postdoctoral fellows from SSAA-supported institutions who join the national laboratories are extremely well prepared to begin their research careers. As a result, the national laboratories are anxious to collaborate with and recruit more individuals from the SSAA.

At this point in time, the SSAA program is very much alive and vibrant, and we are looking forward to the next 20 years.

Happy 20th Year, SSAA!

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

PIs: Professors David A. Hammer (dah5@cornell.edu) and Bruce R. Kusse (brk2@cornell.edu)

The Cornell Center engages in coordinated experimental, theoretical, and computer simulation research on high energy density (HED) plasmas at four U.S. universities and two abroad. The Center experiments investigate the dynamics of HED z-pinch implosions supported by extended magnetohydrodynamics computer simulations using PERSEUS (Cornell) and GORGON (Imperial College) codes. Three current projects are highlighted below.

Zeeman Polarization Spectroscopy (ZPS) is being used to determine the magnetic field profile within gas-puff z-pinch plasmas on the 100-240 ns rise time, 1 MA COBRA pulsed power machine using spectral lines emitted by CO_2 and CO_2-doped neon Z-pinches. ZPS was developed by Center partner, Weizmann Institute of Science on a 500 kA, 500 ns rise time machine.[1] Light is collected parallel to the magnetic field by looking tangentially to the outer edge of the imploding sheath. It is split into left and right circularly polarized components that are delivered independently to a 750 mm spectrometer. A sharp thermal gradient at the sheath edge localizes emission of the spectral lines of interest. The peak emission wavelengths of the two polarizations can be resolved and the local magnetic field determined from their separation despite Stark Broadening, as illustrated in Figure 1.

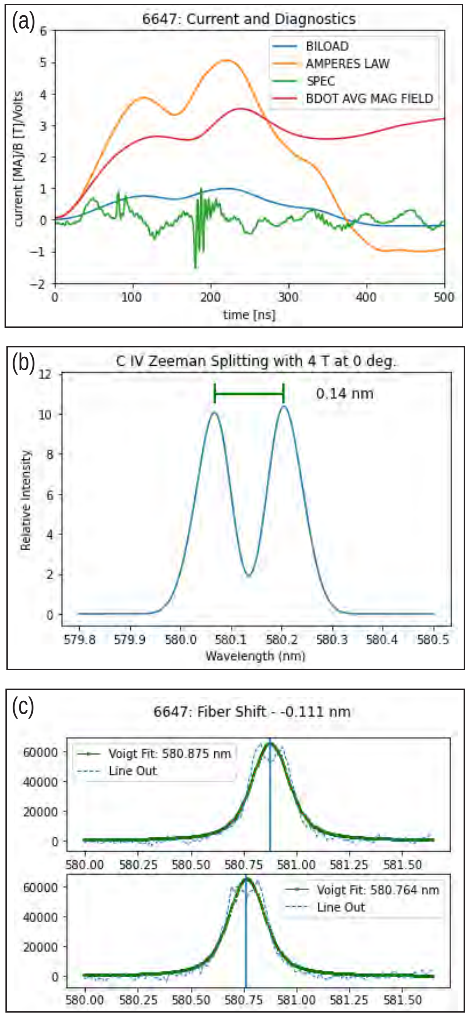

Figure 1. (a) The ZPS measurement in Shot 6647 was made at 185 ns when the current implies a 4 T field and BDOT-probes near the anode gives 2.5 T. (b) A 4 T field splits the C IV doublet line at ~580 nm by 0.14 nm. (c) The ZPS-measured splitting of 0.11 nm gives 3.1T for Shot 6647.

Experiments are underway to understand energy transport throughout a gas-puff implosion. Recent measurements using the full array of COBRA's diagnostics have enabled the calculation of the energy inventory up to stagnation for both axially-magnetized and unmagnetized implosions. The total energy coupled is inferred from machine current and voltage traces while spatially-resolved, plasma parameters such as flow velocity (radial, azimuthal, and turbulent), species temperatures and densities measured at different times over highly repeatable implosions using Thomson scattering (TS) and laser interferometry enable calculation of kinetic and internal energies. Directed, radial kinetic energy also is calculated using implosion models and visible/extreme ultraviolet (XUV) self-emission with a known initial density profile. Radiated energy is measured using a photo-conducting diamond detector (PCD) and bolometer. All of these taken together enable the most comprehensive picture of gas-puff, z-pinch implosion energetics obtained to date, as shown in Figure 2, for an overmatched argon load. At 200 ns, the coupled energy is well accounted for by $E_{total,TS}$. By the end of stagnation, the total energy coupled to the pinch is inferred to be 5.6% of the stored electrical energy. About 11% of the peak radial kinetic energy is in total measured radiation.

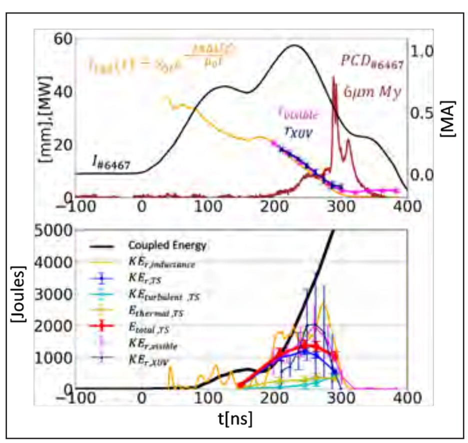

Figure 2. (Top) Representative current trace and radial implosion trajectories. Energies implied by 2/6μm Mylar-filtered radiation detectors are 130/1.4 J. (Bottom) Energy evolution is shown. Error bars are propagated from measurement uncertainties only.

Theoretical work relevant to predicting Warm Dense Matter (WDM) X-ray Thompson scattering (XRTS) spectra is being carried out by Cornell graduate student Thomas Hentschel, working with Sandia National Laboratories Distinguished Member of the Technical Staff, Stephanie Hansen. The inclusion of dynamic electron collision frequencies in free electron models can improve predictions of WDM spectra beyond those from simplified uniform electron gas approximations.[2] Models currently are validated indirectly by finding the one that yields the best fit to experimental data, but large ranges in collision frequencies can correspond to approximately the same predicted spectra. By using Bayesian inference methods, Cornell is exploring if it is possible to extract reliable collision rate information from scattering spectra. This approach could provide a way to directly validate collision models in the WDM regime and to help guide improvements to them.

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[1]G. Rosenzweig, E. Kroupp, A. Fisher, and Y. Maron, JINST 12, P09004 (2017).

[2]A. N. Souza et al., PRE 89, 023108 (2014).

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)

The Massachusetts Institute of Technology (MIT) Center of Excellence is comprised of five partners: MIT, the University of Michigan, the University of Nevada Reno, the University of Rochester, and Virginia Tech. Each of these partners brings a set of unique and complementary capabilities in experiment, theory, and computation and simulation to the Center. With the successful and wide-ranging Center research and PhD programs at OMEGA, the National Ignition Facility (NIF), and Z, the Center generates exceptional experimental and theoretical PhDs in high energy density (HED) physics while addressing issues of great significance to the National Nuclear Security Administration (NNSA) and the national laboratories. Working closely and cohesively together, in collaboration with the national laboratories and the Laboratory for Laser Energetics (LLE), the Center is able to amplify and leverage its impact in the areas of inertial confinement fusion (ICF) and HED physics far beyond that of the individual institutions.

The Center's scientific research programs are comprehensive and challenging, involving the development and application of advanced plasma diagnostics and state-of-the-art experimental platforms, as well as performing theoretical modeling and numerical simulations for exploring a broad range of fundamental physics in the areas of ICF, laboratory astrophysics, and, more generally, HED plasmas. Three and a half years of Center work have led to significant progress in achieving the Center's scientific objectives. This advancement is manifested by a series of notable accomplishments, two of which are highlighted in recent publications in Physical Review Letters (PRL). First is the study of magnetized, shock-driven ICF implosions[1] led by the Center. Second is a NIF ICF ignition experiment achieving recorded fusion yield of 1.35 megajoules that was co-authored by a large number of Center members including PhD students.[2]

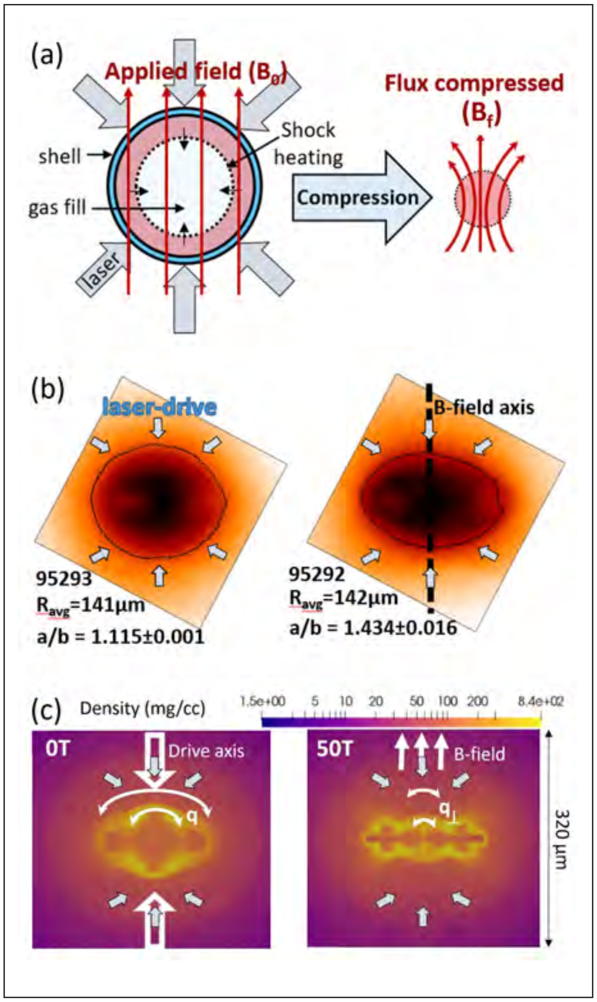

Figure 1. (a) Schematic of the magnetized implosion experiment conducted on OMEGA. (b) X-ray self-emission images of the unmagnetized (left) and magnetized implosions (right). (c) Density profile at bang time from magnetohydrodynamics simulations with 0 kG (left) and 500 kG (right) applied B field. The shorter curved arrows represent a reduced cross field heat flow ($q_\perp$). For details, see PRL.[1]

Figure 1 shows the new experiments at OMEGA, led by Center's postdoctoral fellow, Arijit Bose, reporting the first observation on how a strong, 500 kG, externally-applied, magnetic field increases the mode-two asymmetry in shock-heated, inertial fusion implosions. Using a direct-drive implosion approach with polar illumination and imposed external magnetic field, Dr. Bose and his team observed that plasma magnetization and compression produces a significant increase in the implosion oblateness (a 2.5× larger P2 amplitude in X-ray self-emission images) compared with reference experiments with identical drive but with no field applied. The implosions produce strongly-magnetized electrons ($\omega_e\tau_e >> 1$) and ions ($\omega_i\tau_i > 1$) that, as shown using magnetohydrodynamic (MHD) simulations, restrict the cross-field heat flow necessary for lateral distribution of the laser and shock heating from the implosion pole to the waist, causing the enhanced mode-two shape. The experiment has revealed the effects of magnetic fields on ICF implosion dynamics and has advanced our understanding of plasma magnetization in HED plasmas. This novel work recently has been published in PRL[1] and was selected as Editor's Suggestion and Featured in Physics with a Synopsis[3] for manifesting the importance and significance of this work to a broader PRL readership.

The second PRL article,[2] published most recently and also selected as Editor's Suggestion and Featured in Physics with a Synopsis,[4] reports the game-changing NIF experiment on August 8, 2021 that achieved a record fusion yield of 1.35 megajoules. Sixteen Center members are co-authors along with our colleagues in the ICF community of this seminal PRL paper,[2] including nine outstanding Center PhD students. This co-authorship is a great honor and an acknowledgment of the significant contribution made by Center scientists and students to NIF experiments and to the US ICF program. In particular, the Center-developed Magnetic Recoil neutron Spectrometer (MRS) played a pivotal role for providing measurements of fusion-neutron yields and energy spectra in this ground-breaking experiment.

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Center for Research Excellence on Dynamically Deformed Solids | Texas A&M University

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Following the cessation of nuclear testing in the United States, research directed towards understanding the effects of harsh environmental conditions on components made of metals and alloys became indispensable for maintaining the safety of the stockpile. To meet this challenge, the Center for Research Excellence on Dynamically Deformed Solids (CREDDS) prepares future leaders in stewardship science through fundamental research on advanced metallic materials under mechanical loading conditions at extreme strain rates, pressures, and strains.

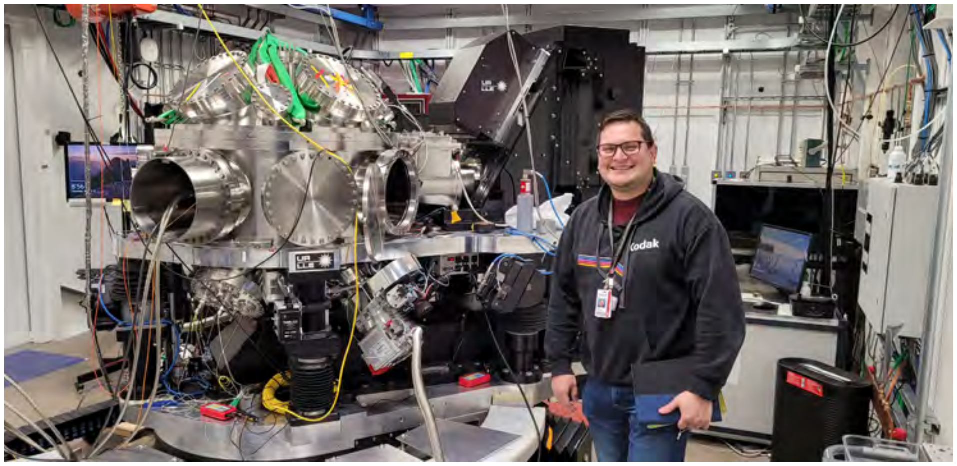


Figure 1. CREDDS PhD student, Marco Echeveria, at DCS.

CREDDS comprises 11 faculty, 17 PhD students, and 4 postdoctoral fellows spread over four institutions: Texas A&M University (lead), University of Connecticut, University of California at Santa Barbara (UCSB), and University of Michigan. Collaborators at the National Nuclear Security Administration (NNSA) laboratories also are key to the mission of CREDDS. They host the Center's graduate students for extended stays at the labs, offering technical mentorship, networking opportunities, and professional insights. During the past fiscal year, six PhD students had internships at NNSA labs. Moreover, three CREDDS alumni transitioned to permanent employment there: PhD graduates, Max Powers and Edwin Chiu, at Lawrence Livermore National Laboratory (LLNL) and Sandia National Laboratories (SNL), respectively, and former postdoctoral fellow, Avanish Mishra, at Los Alamos National Laboratory (LANL). All three previously had forged collaborations with their current employers through CREDDS-supported internships.

For PhD student Marco Echeveria (University of Connecticut), engagement with NNSA staff provides a unique opportunity to perform cutting edge research at the Dynamic Compression Sector (DCS) at the Advanced Photon Source (APS). Working with APS staff directly on site at DCS (Figure 1), Marco—whose background is in atomistic modeling—conducted experiments to test his modeling predictions. By comparing shock-induced changes in diffraction patterns predicted through simulations to ones measured *in situ*, the role of twinning in the mechanical response of body centered-cubic (bcc) metals under high strain rates was elucidated. Marco's findings will advance the development of microstructure-informed constitutive models for the mechanical response of metals with dynamically evolving microstructures.

Figure 2. CREDDS director, Michael Demkowicz, presents undergraduate intern, Victor Villanueva, with an outstanding presentation award from the 2022 O-REU program at Texas A&M University.

Technical collaborations with LANL enabled Lauren Poole, CREDDS PhD student at UCSB, to perform flier plate tests on multi-phase composites of copper (Cu) and tungsten (W). Her findings displayed a marked influence of phase fraction and connectivity on strain-rate-sensitive strength and hardening rates in these materials. Lauren later presented her work at the 2022 Shock Compression of Condensed Matter conference organized by the American Physical Society in Anaheim, California. The excellence of her research was recognized by an early career presenter award.

CREDDS also supported 11 undergraduate researchers over the past year. For many of them, working on a CREDDS project is their first exposure to the stockpile stewardship mission. It is an opportunity to build technical skills and to gain recognition for their accomplishments. For example, Victor Villanueva (pictured in Figure 2), an undergraduate from the University of Virginia, won an outstanding presentation award from the 2022 online Research Experience for Undergraduates (O-REU) program at Texas A&M University for his presentation entitled "Quantitative Metallographic Analysis using Machine Learning." For some of these students, a CREDDS undergraduate internship is a step towards pursuing graduate studies and a future career in stewardship science.

Center for Excellence in Nuclear Training and University-based Research | Texas A&M University

PI: Dr. Sherry Yennello (yennello@comp.tamu.edu); Author: Dr. Lauren McIntosh (centaur@comp.tamu.edu)

The Center for Excellence in Nuclear Training and University-based Research (CENTAUR) collaboration has been supported by the Stewardship Science Academic Alliance (SSAA) since 2018 and currently supports sixteen graduate students and one postdoctoral researcher. These young scientists work at Texas A&M University (TAMU), Florida State University (FSU), Louisiana State University, University of Notre Dame, University of Tennessee-Knoxville, University of Washington-Seattle (UW), and Washington University in St. Louis (WUStL). Seven CENTAUR graduates (over half of our graduates to date) currently work at Lawrence Livermore National Laboratory or Los Alamos National Laboratory (LANL) as either postdoctoral researchers or staff scientists. These students have been educated in low energy nuclear science (experiment and theory) related to the National Nuclear Security Administration mission.

One project is a novel means of neutron detection, a collaboration of TAMU and WUStL personnel. The TexNeut array is a neutron time-of-flight detector.[1] It measures the energy of neutrons that emanate from nuclear physics experiments. The array is made of many individual crystals of a scintillating material called *p*-terphenyl. Highly-sensitive light detection devices called photomultipliers are used to very precisely measure how much light is produced and, more importantly, when the light is produced. In an experiment, nuclear reactions can take place that generate neutrons which then are measured in our detector array. By recording when the reaction happened, the time taken for neutrons to reach the detector is measured. This gives the velocity and, therefore, the kinetic energy of the neutrons detected. The modular design of TexNeut (one module is shown in Figure 1) also allows determination of the exact location of the neutron interaction to a very high fidelity as well as distinguishes between the neutrons of interest and background gamma-ray radiation. TexNeut is used to learn about the properties of nuclei, how different nuclei interact with one another, and about nuclear processes that occur in stars.

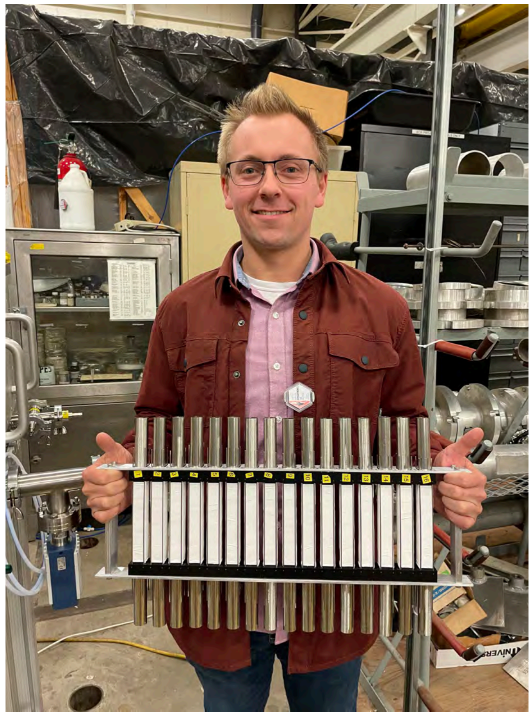


Figure 1. CENTAUR student Dustin Scriven (TAMU) holds newly fabricated bars of TexNeut, ready for its commissioning experiment.

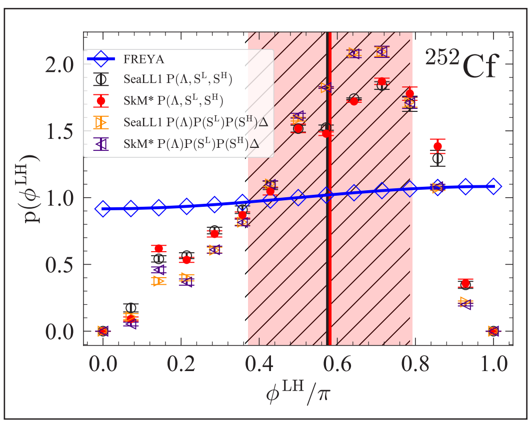


Figure 2. The angle between the fission fragment spins extracted within the microscopic theory with two different density functionals, versus the prediction of the phenomenological model FREYA.[2]

Another project that will enable research to answer similar questions in a different way is the development of a triton beam. Beams of tritium, a radioactive isotope of hydrogen containing one proton and two neutrons, have not been available at accelerator facilities since the 1980s. It is a well-known principle that atomic nuclei contain protons and neutrons moving together in pairs to form their natural ground state, but the degree to which this pairing persists in excited states is much less understood. Accelerated beams of tritium will provide a unique experimental probe to answer this question and provide detailed tests of nuclear theory. Accelerated tritium beams also will provide a valuable resource to study other aspects of stockpile stewardship science. During the last year, the FSU laboratory has built a dedicated injector with a multi-cathode ion source that now has successfully delivered beams of deuterons. Commissioning the facility with tritium is expected in summer 2023.

The time-dependent density functional theory extended to superfluid systems allowed, for the first time, a description without fitting parameters of the non-equilibrium fission dynamics and its strongly damped character, the formation of the fission fragments, their average properties, their total kinetic energy, their excitation energies and the sharing mechanism between the fragments, and the distribution of their spins and their correlations with the relative orbital momentum.[2] One particularly unexpected prediction is the probability distribution of the relative angle between the fission fragment spins, illustrated in Figure 2, which is qualitatively at odds with the predictions of the phenomenological model FREYA.[3] This microscopic calculation has convincingly shown that despite the strong correlation between the fission fragment spins and their relative orbital momentum, the distributions of the fission fragment spin magnitudes are surprisingly independent, in full agreement with experiment[4] but at odds with the interpretation.

References

[1]Scriven et al., Nucl. Instr. Meth. A 1010, 165492 (2021).

[2]Bulgac, Abdurrahman, Godbey, and Stetcu, Phys. Rev. Lett. 128, 022501 (2022).

[3]Randrup and Vogt, Phys. Rev. Lett. 126, 014610 (2021).

[4]Wilson et al. Nature, 590, 142502 (2021).

Center for Matter Under Extreme Conditions | **University of California, San Diego** | PI: Dr. Farhat Beg (fbeg@ucsd.edu)
Authors: Mario Manuel (General Atomics, manuelm@fusion.gat.com) and Tanja Kovacevic (UC, Berkeley, tanja_kovacevic@berkeley.edu)

The Center for Matter Under Extreme Conditions (CMEC) focuses on 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, 13 students from University of California (UC) San Diego, 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. Nine program alumni, including six graduate students and three postdoctoral scholars now work at the DOE/NNSA national laboratories or at General Atomics (GA). Since its inception, CMEC has published over 70 articles in refereed journals. Two recent projects are highlighted below.

Magnetized Collisionless Shocks

Collisionless shocks are ubiquitous in astrophysics and are a possible source of the highest-energy cosmic rays in our universe. Over the last decade, the rise of high-power lasers now provides the means to easily produce high-speed plasma flows (> 1500 km/s) in the laboratory. These high-speed plasmas can be set to collide with a premagnetized, semi-stationary plasma to emulate astrophysical systems, such as supernova remnants, to study the formation of quasi-parallel, magnetized collisionless shocks, which are predicted to be the most efficient source of cosmic rays. However, studying such a process in a laboratory remains challenging, since the instabilities driving the formation of the shock are slow relative to experimental timescales. Nonetheless, the CMEC team successfully visualized the growth of a magnetic field leading to the formation of a parallel shock using a probing proton beam (Figure 1). The dark and light bands are the result of magnetic fields in the plasma that show an increase of magnetic energy with time. The ion-Weibel instability and the Non-Resonant instability (NRI) are identified as the likely generation mechanisms for the observed features. The data suggest that the NRI, also known as the Bell instability, dominates later in time and is usually involved in the magnetic amplification in astrophysical shocks when the cosmic rays travel upstream of the shock.

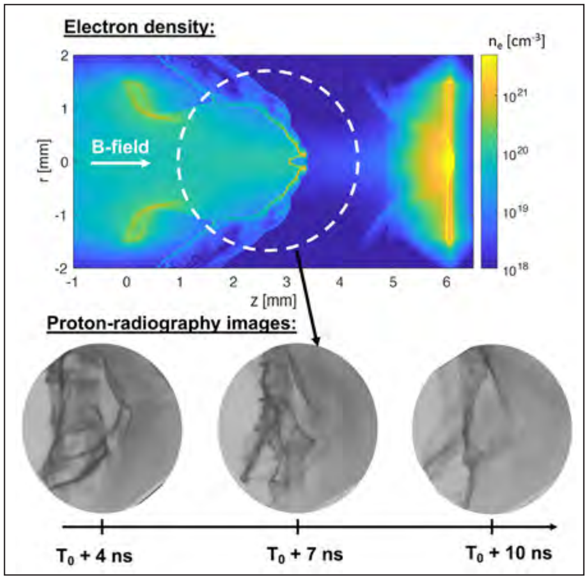


Figure 1. (Top) FLASH-computed electron density distribution for which fast plasma from the right collides with the premagnetized plasma on the left. (Bottom) Results from LaserNetUS experiments executed on the Omega EP laser facility showing the temporal evolution of the electromagnetic field embedded in the plasma visualized with a proton beam. In this collaborative work, experiments were performed by a graduate student, Alem Bogale, postdoc, Simon Bolanos (UC San Diego), and Mario Manuel (GA). Simulations were carried out by postdoc, David Mictha, and Petros Tzeferacos (University of Rochester).

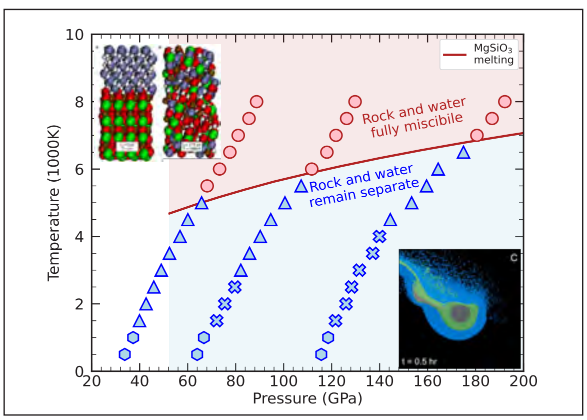


Figure 2. In this collaborative CMEC project, PhD student T. Kovačević in B. Militzer's group, at UCB performed ab initio simulations of rock-ice mixtures (left inset) to determine the conditions for rock and ice mixing (red area) and S. Stewart at UCD conducted impact simulations (right inset) to show that the conditions for mixed rock-ice layers are met during water world formation.

Rock-Ice Miscibility in Water World Exoplanets

The internal structure and evolution of planets are controlled by the thermodynamics of multi-component systems in the HED regime. CMEC investigated the miscibility of rock and icy material for massive water worlds. In this work, they calculated the solidus of a high-pressure rock-ice system and paired our findings with giant impact simulations to provide a proof of concept of mixed mantles within water worlds.

Water worlds are exoplanets more massive than Earth that contain a significant amount of water overlaying a rocky mantle and iron core. Characterizing the interactions between water and rock under the pressures and temperatures within these water worlds is essential to understanding their structure, formation, and evolution. CMEC used density functional theory molecular dynamics to model the dynamics between water and high-pressure $MgSiO_3$, a major silicate phase. They explored pressures ranging from 30–120 GPa and temperatures from 500–8,000 K. The results demonstrate that bridgmanite and water are miscible in all proportions if the temperature exceeds the melting point of $MgSiO_3$ (Figure 2).

Additionally, CMEC performed smoothed particle hydrodynamics simulations to demonstrate that the conditions for rock-water miscibility are reached in the course of giant impacts between water-rich bodies of 0.7–4.7 Earth masses. During this collisional growth of water worlds, rock and water become miscible forming a fuzzy, mixed layer increasing the amount of water incorporated deep within their interiors. This work has been published in Scientific Reports.[1]

Reference

[1]T. Kovačević, F. González-Cataldo, S.T. Stewart, and B. Militzer, *Miscibility of Rock and Ice in the Interiors of Water Worlds*, Sci Rep 12, 13055 (2022).

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)

A key focus area of the Chicago/Department of Energy Alliance Center (CDAC) is plasticity, strength, and deformation of materials at high pressures and temperatures. Experimental and theoretical studies of these properties provide important information on the behavior of materials at extreme conditions and can also address longstanding questions in geoscience.

For example, meteorite impacts are defining events in the evolution of planetary bodies, and an understanding of the conditions generated during an impact event is critical for our knowledge of these processes. Zircon ($ZrSiO_4$) is a orthosilicate found in the Earth's crust and has been used to measure the pressure of, and time since, a meteorite impact. In particular, the presence of twins as well as the high-pressure polymorph of zircon are characteristic of high-pressure shock deformation, but the phase transition and deformation mechanisms still are poorly understood. Theoretical studies predict that the phase transition should begin at approximately 5 GPa, but static and shock experiments document the transition at 20 GPa and 30-40 GPa, respectively. The transition always occurs at higher pressure during shock compared to static compression, suggesting that strain rate may play an important role in the phase transition.

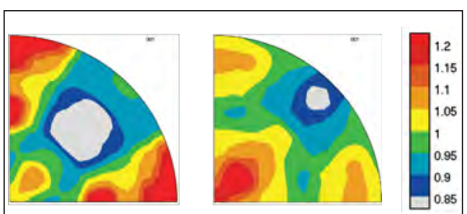
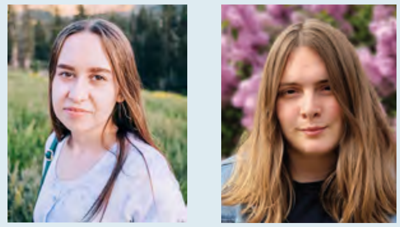


Figure 1. Inverse pole figures in the compression direction [001] for zircon at 32 GPa. Left, dynamic compression; Right, static compression. The color scale represents multiples of the random distribution, with redder colors indicating greater texture development.

Material deformation during a meteorite impact is estimated to occur at strain rates of 10^2 to 10^3 s^{-1}. Static and shock techniques achieve strain rates that are too low (static) and too high (shock) to document changes in material properties with sufficient resolution. To address this question, graduate student



CDAC graduate students Chantelle Kiessner (University of Utah) and Allison Pease (Michigan State University).

Chantelle Kiessner, from the group of CDAC academic partner Lowell Miyagi at the University of Utah, uses the radial dynamic diamond anvil cell (rdDAC), a technology developed with CDAC support, at the Deutsches Elektronen-Synchrotron (DESY) PETRA III facility in combination with time-resolved X-ray diffraction. A comparison of results from static and rdDAC experiments shows that texture evolution depends sensitively on the strain rate (Figure 1). Further work is addressing the effects of radiation damage from the radioactive decay of uranium in natural zircon on phase transition pressures and other physical properties.

Geophysical observations indicate that seismic waves in Earth's inner core travel faster in the north-south than in the east-west direction, indicative of preferred orientation in iron/alloy crystals induced by either plastic deformation or crystal growth. It is thought that nitrogen in Earth's core could facilitate the formation of lattice preferred orientation. The strength of these materials not only depends on composition but also the extreme temperature and pressure conditions found during mechanical impacts and in planetary interiors.

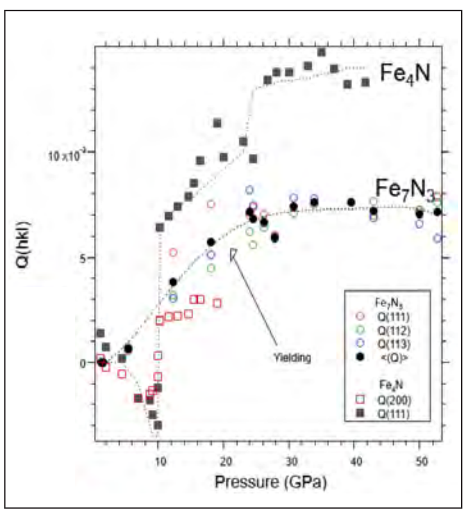


Figure 2. Elastic strain, represented by Q (hkl), as a function of pressure for iron nitrides. Q (hkl) is determined for different diffraction peaks.

To determine the strength, deformation behavior, and electronic properties of Fe-N alloys at high pressures, CDAC graduate student Allison Pease, from the group of academic partner Susannah Dorfman at Michigan State University, uses X-ray diffraction and X-ray spectroscopy to investigate iron nitrides at high pressure. Whereas X-ray diffraction is used to observe elastic and plastic strain and determine the yield strength, X-ray emission spectroscopy provides the total electronic spin moment of iron. Results demonstrate that the onset of a high- to low-spin transition in Fe (10 GPa and 5 GPa for ε-Fe_7N_3 and γ-Fe_4N, respectively) precedes yielding in the iron nitrides at 17 GPa (ε-Fe_7N_3) and 9 GPa (γ-Fe_4N). Below these pressures, the nitrides deform elastically, and at higher pressures each material exhibits a mixture of plastic and elastic deformation (Figure 2). Ongoing investigations are examining the effects of high temperatures on the deformation behavior of these materials to evaluate the possibility that they may be hosts for the light alloying element in Earth's core (Figure 3).

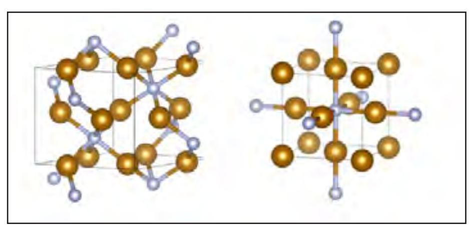


Figure 3. Crystal structures of ε-Fe_7N_3 (left) and γ-Fe_4N (right). Gold spheres, Fe; silver spheres, N.

The Center for Laboratory Astrophysics | University of Michigan

PI: Dr. Carolyn Kuranz (ckuranz@umich.edu)

The Center for Laboratory Astrophysics (CLA) studies high energy density (HED) science relevant to astrophysical phenomena in three main areas: Radiation Hydrodynamics, Complex Hydrodynamics and Hydrodynamic Instabilities, and Magnetized Flowing Plasmas. Whereas the main work of CLA is experimental with experiments performed at a variety of high energy density (HED) facilities, the Center also performs radiation hydrodynamic simulations using the CRASH code, a multigroup, flux-limited diffusion, radiation hydrodynamics code. The Center currently has nine graduate students and two postdoctoral fellows. CLA students often work closely with scientists and engineers at the National Nuclear Security Administration (NNSA) laboratories and facilities as part of their doctoral work. CLA hosted the 2022 High Energy Density Summer School, which is open to the HED community. University of Michigan Professors Baalrud, McBride, Johnsen, Kuranz, Krushelnick, Willingale, and Dr. Heath LeFerve gave lectures about the theoretical underpinnings of HED science.

Specifically, for their complex hydrodynamics work, CLA researchers' study the Kelvin Helmholtz (KH) instability relevant to early galaxy formation in the Universe. Hydrodynamic instabilities commonly occur in astrophysical systems due to density and velocity and/or pressure gradients often generated by shock waves. Additionally, inertial confinement fusion (ICF) experiments also have multiple shocks that traverse material interfaces where complex instabilities and mixing can develop, injecting cold material into the central hot spot which reduces the fusion yield. According to Dr. Carolyn Kuranz, the Center Director and an Associate Professor at the University of Michigan, "CLA researches fundamental HED science that is relevant to astrophysical systems and the Stockpile Stewardship Program."

CLA designed an astrophysically-scaled experiment on Omega EP that explores the KH instability under conditions relevant to early galactic formation.[1] The Universe is a cosmic web that is composed of filaments and galactic halos. Filaments are cold and dense "cylindrical streams" of dark matter and mass. Halos are "spherical clumps" of dark matter in the center of which galaxies form. Galaxies grow by accreting gas from the halos, and the stars that form within the galaxies are regulated by the availability of the gas. In essence, the gas supply to the galaxy acts as a bottleneck for star formation and ultimately sets its star formation rate. It is known that the most productive star-forming galaxies in the universe were young (redshift z ~ 2.5) and had a mass (M) of ~ 10^{11} solar masses. It is speculated that these galaxies were stream-fed by filaments.

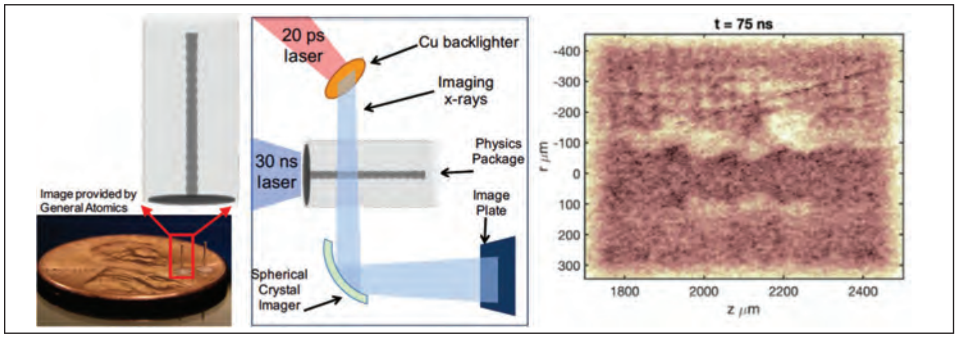


Figure 1. (Left) Schematic of experiment on Omega EP and X-ray radiograph of KH instability growth. Figure prepared by Adrianna Angulo.

Galactic Cold Stream and Experiment

Parameter	Symbol	Cold Stream	Experiment
Hydrodynamics:			
Localization	l_c/h	1.8×10^{-5}	4.9×10^{-6}
Ryutov number	$\tilde{v}\sqrt{\tilde{\rho}/\tilde{p}}$	2.2	2.3
Heat transport:			
Thermal diffusivity ($cm^2\ s^{-1}$)	χ	2.4×10^{26}	5.1
Peclet number	Pe	2.5×10^3	6.0×10^3
Momentum transport:			
Thermal viscosity ($cm^2\ s^{-1}$)	ν	3.2×10^{24}	4.4×10^{-2}
Reynolds number	Re	1.9×10^5	6.8×10^5
Radiation:			
Compton mfp (cm)	l_{rad}	1.3×10^{26}	41
Cooling time	$\tau_{cooling}/\tau$	2.3	...

Table1. Derived Scaling Parameters for the Galactic Cold Stream and Experiment. For more details, see reference 1.

However, the cosmological-scale simulations capable of resolving the filaments only captured large-scale structure and failed to resolve the dissipative processes that occurred along the filament boundary. The cold, dense filament and its surrounding gas, which is warmer and less-dense, have differing velocities. The velocity difference present on the filament boundary implies that the system is KH unstable. Therefore, experiments that capture the KH behavior can help determine the rate at which hydrodynamic effects contribute to the dissipative process.

Figure 1 shows a schematic of the target design. The target consists of a thin, plastic ablator and preheat shield followed by a narrow (200 μm diameter) plastic rod of density ρ_{rod} = 1.4 g cm^{-3} inserted in the center of the low-density foam cylinder of density ρ_{cyl} = 140 mg cm^{-3}. The CHI rod is relatively opaque compared to the PAI to the backlighter source (either Cu or Mn at 8.0 keV or 6.1 keV, respectively). The laser irradiates the 50 μm ablator using three sequential 10 ns pulses to create a strong shock that propagates through the shock tube. The shock travels faster in the foam than the rod, and the resulting shear creates a KH-unstable system. The surface of the rod is modulated with a single-mode sine wave of wavelength 100 μm and a peak-to-valley amplitude a = 10 μm to seed the KH instability along the interface. The experiments used a Spherical Crystal Imager to create a high-resolution, high signal-to-background radiograph of the KH instability growth (Figure 1). CLA has completed the experimental design using a radiation hydrodynamics codes and astrophysical theory. They currently are analyzing experimental data and refining radiation hydrodynamics simulations. The experimental and computational work was performed by CLA graduate students Adrianna Angulo and Shane Coffing, respectively.

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Actinide Center of Excellence | University of Notre Dame

PI: Dr. Amy E. Hixon; Author: Kelsey Anderson (kander43@nd.edu)

The term actinides refers to the row of the periodic table containing elements with atomic numbers 89 through 103 (actinium through lawrencium). All actinides are radioactive and considered 5f elements. There are wide-ranging uses for these elements but perhaps most relevant here are their applications in nuclear power and weaponry. Elements such as uranium and plutonium are especially important given the composition of the Nation's nuclear weapons stockpile. For these reasons, the Actinide Center of Excellence (ACE) was founded in 2017 to investigate research questions relating to actinide chemistry and materials as they apply to national security and stockpile stewardship. This research probes materials in both solution and solid state using experimental and computational methods.

ACE consists of 7 senior investigators, at least 12 PhD students, and 3 postdoctoral scholars across five universities and is funded through a cooperative agreement with the National Nuclear Security Administration's (NNSA's) Stewardship Science Academic Alliance (SSAA) program. Because ACE focuses on answering fundamental science questions regarding actinides and their application to stockpile stewardship, its breadth is vast, leading students to study a multitude of different, but relevant topics. These range from synthesis of new actinide metal–organic frameworks[1] and examination of actinide and lanthanide metal-oxo clusters[2] to probing actinide materials under extreme conditions like irradiation[3] and high pressure, the latter of which is one of ACE's most recent forays.

Due to the safety concerns that are inevitable when investigating actinide materials, the field of high pressure actinide research is limited but growing. Research of actinide materials under extreme conditions is especially important, because it has the potential to reveal information that can increase the reliability and safety of the stockpile and perhaps even influence the design of future weapons programs. Through the use of a static diamond anvil cell (DAC), researchers are able to insert a sample between two diamonds (Figure 1), increase pressure by tightening screws or introducing an inert gas via membrane, and then measure changes in coordination geometry, electronic properties, and structure axially (through the diamond) or radially (through a Be gasket, which is X-ray transparent). Internal pressure can be determined through the inclusion of ruby spheres in the sample and measured by chromium fluorescence via Raman spectroscopy (Figure 2).

Figure 1. Kelsey Anderson checking that the DAC is sealed.

Thanks to the NNSA's High Pressure Collaborative Access Team (HPCAT) beamlines at the Advanced Photon Source, ACE researchers have been able to perform experiments using X-ray absorption spectroscopy (XAS), a synchrotron-based technique, that can be performed on crystalline or amorphous materials in order to determine oxidation state and local bonding environment (i.e., short-range order). These experiments were used to study a variety of uranium-containing compounds such as uranium dioxide ($U^{IV}O_2$), the material most commonly used for nuclear fuel, and studtite ($[(U^{VI}O_2)O_2(H_2O)_2]\cdot 2H_2O$), a naturally occurring uranyl peroxide mineral. Preliminary studies suggest a reduction in the oxidation state of uranium occurs with increasing pressure in both of these materials. Even more specifically, at pressures greater than 7.4 GPa—similar to pressures experienced deep in the Earth's asthenosphere—studtite appears to lose its axial oxygen (i.e., uranyl) bonds in favor of a uranate-like configuration. This is interesting given the rarity of the uranate-like configuration and the common presumption that U(V) is a metastable oxidation state and provides an opportunity to probe the electronic structure of U(V) using other characterization techniques.

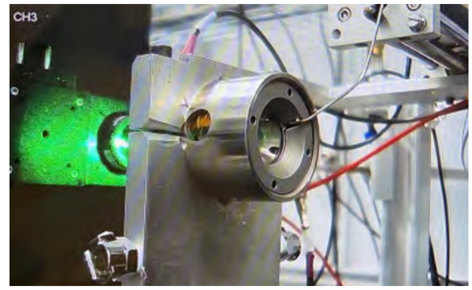

Figure 2. View of DAC in the axial position to measure internal pressure at HPCAT's 16-BM-D beamline.

In addition to the aforementioned reasons for exploring changes in actinide materials under pressure, this work affords students valuable cross-training in the handling of radioactive materials and analysis using synchrotron-based X-ray techniques to which they may not otherwise have access. Such techniques include XAS, X-ray emission spectroscopy, and X-ray diffraction. Familiarization with these methods, even outside of high-pressure research, helps prepare students for careers at the NNSA laboratories because these skills are so highly valued.

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The 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 to explore in the laboratory matter under a wide variety of cosmic conditions, transforming astrophysics into experimental science. WCAPP enables graduate students and postdoctoral researchers to work in a national laboratory scientific culture and to gain expertise in theoretical and experimental atomic physics, spectroscopy, and platform development. Fundamental science experiments are conducted on the Z Pulsed Power Facility (Z) at Sandia National Laboratories (SNL) and at the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory. At present, WCAPP carries out four independent, astrophysically-motivated experiments simultaneously on each shot on Z. There have been three shot series on Z and one shot series on NIF in the past year; each has led to significant progress on all of our experiments.

Over the past year, the white dwarf team has made experimental and theoretical advances in our understanding of the fundamental properties of white dwarf stars. Marc Schaueble (former graduate student, now SNL staff) led the publication of results for helium experiments addressing untested physics used in the spectral models of helium-atmosphere white dwarfs.[1] He found that He I Stark broadening models used in analyses are accurate within errors at tested conditions. Thus, the disagreement in masses derived from spectroscopic versus photometric fits of these stars is most likely not due to the assumed atomic physics. In addition, Patty Cho (Figure 1) led the publication of a new generation of hydrogen line calculations covering a range of temperatures and densities.[2] Postdoctoral researcher, Bart Dunlap (Figure 1), has led platform development efforts on the white dwarf gas cell resulting in successfully using optical light from the Z-pinch as a brighter backlight source for absorption measurements. He has modified the platform to reliably measure H Balmer spectra at higher densities and, based on the success of the University of Nevada Reno (UNR) team using photonic Doppler velocimetry (PDV), he has fielded the first shots using PDV as an independent electron density diagnostic.

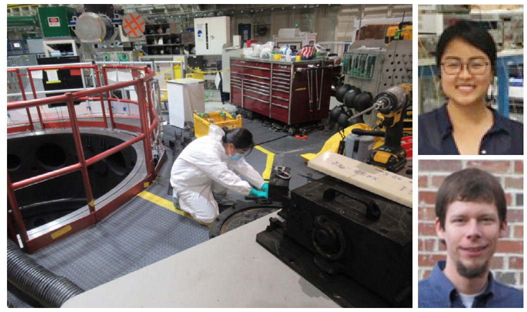

Figure 1. Senior graduate student and Laboratory Residency Graduate Fellowship (2020-2022) awardee, Patty Cho (left and upper right), at work near the center section of the Z machine. WCAPP postdoctoral researcher and team leader of the white dwarf experiment, Bart Dunlap (lower right).

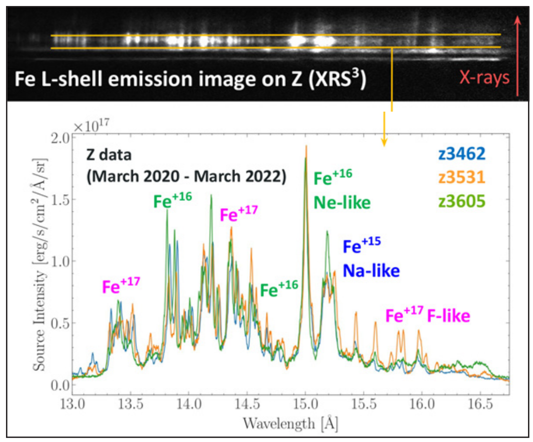

Figure 2. First-ever laboratory measurements of Fe L-shell emission from a photoionized plasma.

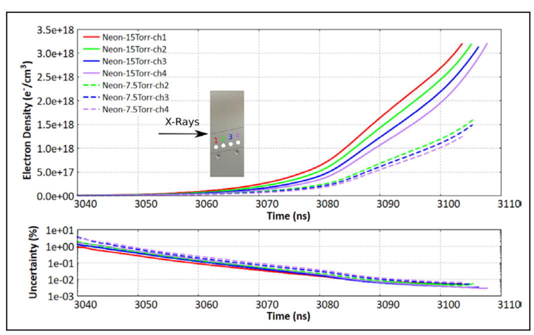

Figure 3. Spatially-resolved electron density time histories measured by four and three PDV probes fielded with 15 Torr and 7.5 Torr neon gas fill pressures, respectively, in the photoionized plasma gas cell experiment at Z. The schematic shows the four probe locations along a 12 degree line-of-sight through the gas cell. The depth of the gas cell is 1.15 cm.

The Accretion-Powered Photoionized Plasma experiment explores the conditions in accreting material around compact objects, such as black holes or neutron stars, where copious amounts of X-rays are generated. The Z facility recreates the relevant state of X-ray photoionization of the radiation-dominated disk environment. We observe spectral emission and absorption from plasmas analogous to those found in astrophysical settings.[3] One long-standing puzzle in astrophysics is that observations of Fe abundances in black hole accretion disks are much higher than expected. Recently, Guillaume Loisel, Patricia Cho, and their team used Z to collect the first-ever laboratory measurements of Fe L-shell emission from a photoionized plasma at astrophysical conditions (Figure 2). These data will help inform any systematic modeling errors that could lead to incorrectly inferred Fe abundances.

Recent progress has been made to develop a novel application of PDV as a plasma electron density diagnostic on radiation science experiments at Z relevant to astrophysics.[4] This was pioneered by UNR graduate student, Kyle Swanson, on the photoionized plasma gas cell platform at Z as part of his PhD dissertation research. This diagnostic provided the first temporally- and spatially-resolved electron density measurements in the gas cell across the duration of the experiment while in the high X-ray flux environment of Z. These measurements allowed, for the first time, a direct observation of the formation and time-evolution of the photoionized plasma in the gas cell as well as a quantitative assessment of the spatial extent and uniformity of the hydro-unperturbed region in the gas cell as predicted by radiation-hydrodynamic simulations (Figure 3). The existence of this region is a critical feature of the photoionized gas cell experiment. The success of this diagnostic in the gas cell platform has led to PDV being implemented on other laboratory astrophysics gas cell platforms at Z such as the white dwarf photosphere and the photoionization front experiments.

References

[1]Schaeuble et al., ApJ 940, 181 (2022).
[2]Cho et al., ApJ 927, 70 (2022).
[3]Loisel et al., PRL 119 (2017).
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Measurements of Prompt Neutron Differential Multiplicity in Photon-Induced Fission | Duke University

PI: Dr. Calvin R. Howell (howellc@duke.edu)

Nuclear fission is the primary energy-producing reaction in critical assemblies. Detection and analysis of the prompt fission neutron spectra (PFNS) from active beam interrogation provide important diagnostics about the fissile and fissionable nuclei in the assembly. Duke University is performing the first differential neutron multiplicity measurements of the PFNS as a function of neutron energy and angle for photon-induced fission with a nearly mono-energetic beam. These measurements are carried out using a pulsed, circularly-polarized, gamma-ray beam from the High Intensity Gamma-ray Source (HIγS) at the Triangle Universities Nuclear Laboratory (TUNL). This work is supported by the Stewardship Science Academic Alliances program and is conducted by a collaboration of groups from Duke University, Lawrence Livermore National Laboratory, and Los Alamos National Laboratory. Two graduate students and a postdoctoral fellow currently are supported by this grant. Collin Malone was a graduate student working on this project to gain expertise in time-of-flight (TOF) spectroscopy of fast neutrons. He received his PhD from Duke University during the summer 2022 and now is a postdoctoral fellow at the Savannah River National Laboratory.

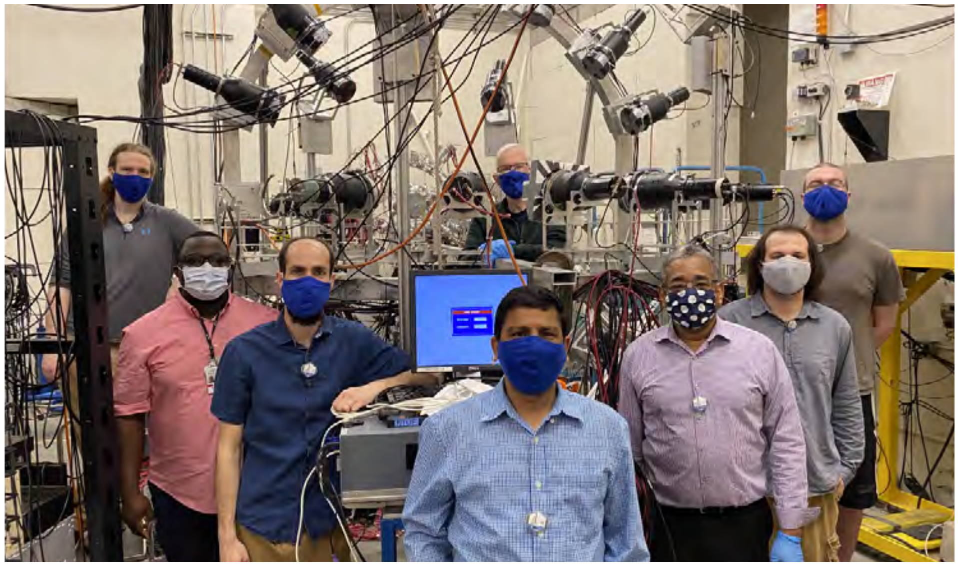

Figure 1. Photograph of experimental setup for the measurements of prompt neutrons emitted in photon-induced fission at HIγS. The neutrons are detected in the array of liquid scintillators that surround the target. The energies of the detected neutrons are determined via TOF measurements. Pictured (left to right) are members of the Duke research team: Forrest Friesen (Postdoc), Innocent Tsorxe (Graduate Student), Sean Finch (Research Scientist), Krishichayan (Research Scientist), Calvin Howell (PI), Ethan Mancil (Graduate Student), Collin Malone (Graduate Student), and Werner Tornow (Senior Investigator).

A photograph of the experimental setup with the Duke group is shown in Figure 1. The technique is based on tagging the fission fragments using a dual fission chamber (DFC).[1] The measurements for ^{235}U, ^{238}U, and ^{239}Pu are performed simultaneously using three DFCs, one for each isotope with each DFC containing two foils of the same isotope. The signal from each DFC provides a time reference for fission events and the pulse height of the energy deposited by the fission fragments in the P-10 chamber gas. The neutrons are detected in an array of 30 liquid organic scintillators in coincidence with the fission event time reference derived from DFC signals. This technique excludes neutrons from the (γ, n) and (γ, 2n) reaction channels. Each scintillator cell is cylindrical with an active volume of 5-inch diameter × 2-inch length and is filled with BC-501A (or equivalent) scintillator fluid. The center-to-center distance between each neutron detector and the DFC is 100 cm. The neutron angular distribution is measured over the reaction angle range from 22.5° to 157.5° in 22.5° steps. The gamma-ray beam pulses are separated by 179 ns and have a width of 0.3 ns full width at half maximum (FWHM). The TOF of the detected neutrons is measured relative to the accelerator radio frequency (RF) signal, and the neutron energy is computed from the measured TOF. The data are analyzed with neutron detector thresholds set to 44 keVee, which corresponds to about 0.5 MeV neutron energy. The energy spectra are fitted with a Watt spectrum assuming 0.4 MeV/nucleon fragment kinetic energy. Measurements have been performed at gamma-ray beam energies of 11.2 and 13.5 MeV. The angular differential neutron multiplicity data for photofission of ^{235}U at 13.5 MeV is shown in Figure 2. There is a slight fore-aft angular asymmetry in the differential multiplicity with a larger number of neutrons emitted to backward angles than to forward angles. A fore-aft angular asymmetry in the differential neutron multiplicity is also observed in the photofission of ^{238}U and ^{239}Pu but is smaller in magnitude than for ^{235}U.

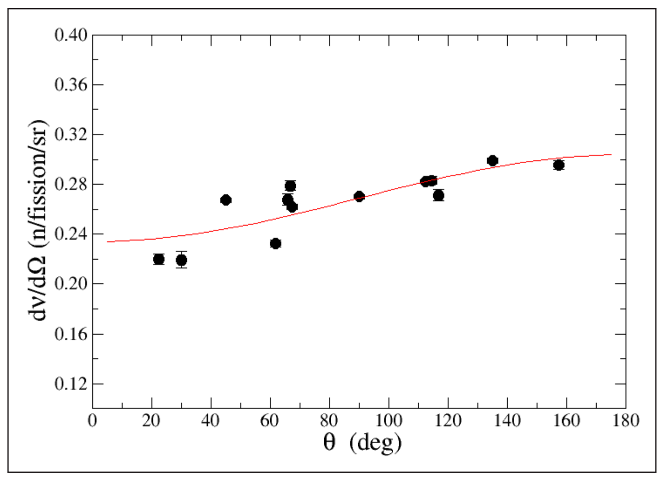

Figure 2. Plot of the data for the angular differential neutron multiplicity for ^{235}U(γ, fn) at E_γ = 13.5 MeV. The error bars on the data points represent the statistical uncertainty only. The curve is a fit to the data with the function $d\nu/d\Omega = a + b\cos(\theta)$. The average value of the neutron multiplicity determined from these data is ν = 3.38 ± 0.20. These results are preliminary.

Reference

[1]M.E. Gooden et al., *Energy Dependence of Fission Product Yields from 235U, 238U and 239Pu for Incident Neutron Energies Between 0.5 and 14.8 MeV*, Nuclear Data Sheets 131, 391 (2016).

Measurement of Fission Product Yields from ^{239}Pu | Duke University

PIs: Dr. P.W. Tornow (tornow@tunl.duke.edu) and S.W. Finch (sfinch@tunl.duke.edu)

Nuclear fission is the process in which a nucleus splits into two fragments and releases a large amount of energy. This process is central to the applications of nuclear energy and stockpile stewardship. Hundreds of different fission products can be produced following fission. The probability that a certain nuclide is produced is known as the fission product yield (FPY) and is one of the key observables of the fission process. A collaboration between Triangle Universities Nuclear Laboratory (TUNL), Lawrence Livermore National Laboratory (LLNL), and Los Alamos National Laboratory (LANL) is producing high-precision measurements of cumulative fission product yields. Members of the collaboration are shown in Figure 1. Duke graduate student, Aitor Bracho, recently has joined the research group. This work is supported under the Stewardship Science Academic Alliance program under grant number DE-NA0003884.

Figure 1. Members of the TUNL-LLNL-LANL experimental collaboration in the TUNL tandem control room. From left to right: S.W. Finch (Duke), W. Tornow (Duke), J.A. Silano (LLNL), M.E. Gooden (LANL), J.B. Wilhelmy (LANL), A.P. Tonchev (LLNL), and A.P.D. Ramirez (LLNL).

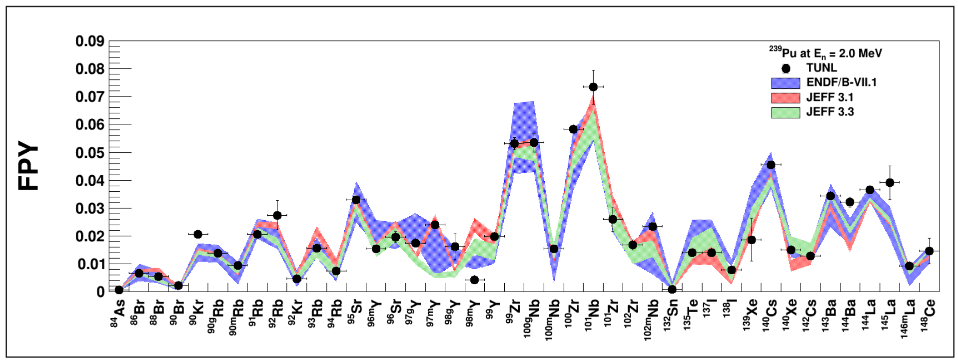

Figure 2. Measured FPYs for ^{239}Pu following fission with 2.0 MeV neutrons. The data is compared to the ENDF/B and JEFF evaluations for fission induced by fission-spectrum neutrons.

Fission products cover a wide range of half-lives from 100 ms to decades. The products with half-lives less than five minutes can be difficult to experimentally measure, as often they will decay before measurement. To gain access to these fission products, the collaboration built a RApid Belt-driven Irradiated Target Transfer System (RABITTS)[1] which is installed at the TUNL tandem laboratory. This system moves a target between an irradiation position, located along the neutron beam axis and near the neutron production source, and a gamma-ray counting station in an adjacent room. The counting station is comprised of two, broad-energy, germanium detectors. The RABITTS moves the target 7.7 m in 1.05 s, reaching a top speed of 10 m/s. This fast transit time enables measurements of fission products with half-lives down to 0.8 s. Once the target is in the counting station, fission products can be identified and quantified by measuring the energy of the emitted gamma rays and the half-life characteristic of their decay.

The collaboration is measuring fission product yields for ^{235}U, ^{238}U, and ^{239}Pu. A plot of measured fission product yields for ^{239}Pu, following fission induced by 2.0 MeV neutrons, is shown in Figure 2. The data is compared to the ENDF/B and JEFF evaluations for fission-spectrum neutrons, a broad energy spectrum with an average energy of 0.5 MeV. The present data shows a considerable reduction in the uncertainty compared to the evaluations. By utilizing the mono-energetic neutron beam available at the TUNL tandem accelerator, scientists can study how fission product yields evolve as a function of the incident neutron energy. Prior to this work, evaluations only were performed for three broad neutron energies. The TUNL-LLNL-LANL collaboration has taken data at five discrete neutron energies, considerably expanding the available database for studying the energy-dependence of the FPYs. These data are necessary to help guide new theoretical models of the fission process.

The present data also is of interest for the reactor antineutrino spectral anomaly. Neutrino experiments recently have observed an excess of 4.5-6 MeV antineutrinos compared to state-of-the-art reactor models. There only are a few fission products that can produce antineutrinos in this energy range with the required intensity. The RABITT system allows direct access to measure these FPYs of interest. The newly measured FPYs then can be incorporated into predictions of the reactor anti-neutrino spectra. Aitor Bracho will be exploring this topic as part of his PhD thesis.

Reference

[1]S.W. Finch et al., *Development of a Rapid-Transit System for Precision Nuclear Physics Measurements*, Nucl. Instrum. Meth. A 1025, 166127 (2022).

Thermodynamic and Mechanical Properties of Stockpile Stewardship Program Materials from Simultaneous Ultrasonic and X-ray Studies at High Pressure and Temperature | Stony Brook University

PIs: Baosheng Li (baosheng.li@stonybrook.edu), Robert C. Liebermann (robert.liebermann@stonybrook.edu)

The ultrasonics group led by Drs. Baosheng Li and Robert C. Liebermann at Stony Brook University conducts basic research on physical properties of materials under extreme conditions of pressure and temperature. Since 2006, the Stewardship Science Academic Alliance (SSAA) has been supporting the ultrasonics group to investigate the thermodynamic and mechanical properties of transitional metals and lanthanides such as equation of states, sound velocities, bulk and shear moduli as well as bulk mechanical properties at extreme conditions that constitutes a critical component of the Stockpile Stewardship Program. The SSAA program at Stony Brook University engages graduate students and postdoctoral associates in research in fundamental science that trains students for the National Nuclear Security Administration (NNSA) mission. One student currently is supported by the SSAA program. Over the past years, two program alumni have accepted positions at the national laboratories, including a Seaborg Postdoctoral Fellow at Los Alamos National Laboratory (LANL).

Simultaneous ultrasonic interferometry and X-ray diffraction measurements at high pressure and high temperature in the multi-anvil apparatus (Figure 1) offer a unique, state-of-the art technique for precise and complete investigation of thermodynamic and mechanical properties. Specifically, shear rigidity can be measured together with bulk modulus by measuring the sound velocities using ultrasonic methods at the same conditions, while the density equation of state is determined using the X-ray diffraction. To support the NNSA mission, the ultrasonics group at Stony Brook University has applied this advanced technique to a range of selected transition metals and lanthanides, including molybdenum, tungsten, zirconium, niobium, neodymium, praseodymium, as well as a range of earth materials.[1] These research projects involve measurements of sound velocities and densities to construct equations of state as well as detect and interpret the governing physics for anomalies across their phase transitions at high pressures. This technique has

Figure 1. The 2000-ton, multi-anvil, high pressure apparatus installed in the High Pressure Lab at Stony Brook University.

been implemented and has become available for general users at nearly all major synchrotron X-ray sources, including an installation at Sector 16 of the High Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source. This has enabled an ultrasonics group alumnus working at LANL to conduct simultaneous ultrasonic and X-ray studies on high pressure elasticity and thermal properties of depleted uranium.[2] NNSA projects at Stony Brook University also involve understanding the macroscopic stress based on the experimentally-derived data to access the bulk yield strength of materials. Another major goal of the project aims to push the envelope of elasticity measurements to higher pressures to reduce the pressure gap between static measurements and shock wave experiments for more reliable interpretation of shockwave data and calculation of properties along shock Hugoniots.

In the past year, PhD student, Siheng Wang, conducted measurements on iron and iron-nickel alloys.[3] Sound velocities of iron and iron-nickel alloys at high pressure and high temperature are of crucial importance not only for fundamental science in condensed matter physics, but also for understanding the composition and structure of Earth's and other telluric planetary cores. Using a multi-anvil apparatus installed at Stony Brook University (Figure 1), Siheng Wang performed ultrasonic velocity measurements on a range of Fe(1-x)

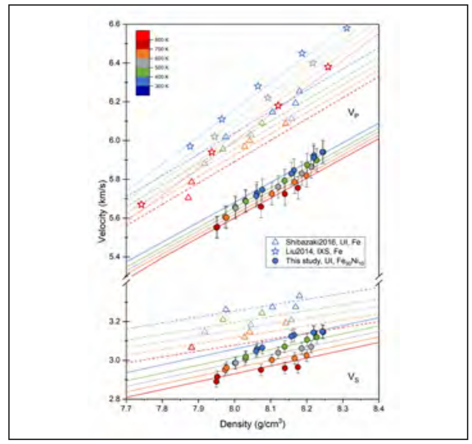

Figure 2. Compressional (VP) and shear (VS) wave velocities as a function of density and temperature for $Fe_{90}Ni_{10}$. Solid lines are the fitting curves from this study. Dashed lines are calculated from Ref. 4, and dotted lines are calculated from Ref. 5.

Ni(x) compositions (x=0, 10, 20, 34), and the results for the compressional and shear velocities of cubic-$Fe_{90}Ni_{10}$ up to 8 GPa 773 K are presented in Figure 2. The bulk and shear moduli as well as their pressure and temperature derivatives were determined precisely by a least-square fit of the data (Figure 2) to finite strain equations. These direct measurements illustrate that alloying with nickel not only decreases sound velocities of iron but also greatly weakens the temperature effects on its elastic bulk and shear moduli.[3]

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[2]M.K. Jacobsen and N. Velisavljevic, *High Pressure Elasticity and Thermal Properties of Depleted Uranium*, Journal of Applied Physics 119, 165904 (2016). doi.org/10.1063/1.4948300

[3]S. Wang, N. Cai, X. Qi, S. Chen, and B. Li, *Sound Velocities of Iron-nickel (Fe90Ni10) Alloy Up to 8 GPa and 773 K, The Effect of Nickel on the Elastic Properties of bcc-iron at High P-T*, American Mineralogist 106, 1744–1750 (2021).

[4]Y. Shibazaki et al., *Compressional and Shear Wave Velocities for Polycrystallinebcc-Fe Up to 6.3 GPa and 800 K*, American Mineralogist 101, 1150-1160 (2016). doi: 10.2138/am-2016-5545.

[5]J. Liu, J. F. Lin, A. Alatas, and W. Bi, *Sound Velocities of bcc-Fe and Fe0.85Si0.15 Alloy at High Pressure and Temperature*, Physics of the Earth and Planetary Interiors, 233, 24-32 (2014). doi: 10.1016/j.pepi.2014.05.008.

Novel Techniques for the Production of Robust Actinide Targets | University of Notre Dame

PI: Ani Aprahamian (aapraham@nd.edu)

The Stewardship Science Academic Alliance (SSAA) supports a research project at the University of Notre Dame (ND) to investigate novel approaches in the preparation of actinide targets. The project team consists of the Principal Investigator, Ani Aprahamian, Freimann Professor of Physics and Astronomy, Associate Research Professor, Khachatur Manukyan, and Dr. Ginger Sigmon.

Thin, isotopically-pure, actinide targets are vital for nuclear science and stockpile stewardship. Actinide targets prepared by conventional techniques have a low stability and consume a considerable quantity of expensive and hazardous radioactive materials. This project already has developed ground-breaking, new approaches for the preparation of actinide targets with controlled thicknesses and a very efficient use of materials.

This work relies on solution combustion synthesis (SCS) reactions between actinide metal nitrates with organic compounds. They investigate the chemical mechanism of SCS reactions to prepare actinide oxides. They use a large array of spectroscopic and imaging methods to reveal the dynamics of combustion processes and ways to control the characteristics of the products. They now understand actinide oxide formation within rapid exothermic processes and use combustion synthesis to deposit thin targets on different backings. The group uses spin coating, spraying, or inkjet printing to deposit thin, combustible solution layers on a variety of substrates, followed by short duration (15 minutes) heating in a furnace at 300-500°C. This is shown in Figure 1. These procedures provide precise control over the target thicknesses and high efficiency in the use of minimal amounts of radioactive materials. The team takes advantage of the accelerator facility at the ND Nuclear Science Laboratory to investigate the irradiation of prepared targets. Tests show that target layers do not disintegrate or lose adherence to the backings even with large energy and intense exposure (1-2 MeV Ar beams and fluences of 10^{17} ions/cm^2).

The project has resulted in extensive collaborations with Oak Ridge National Laboratory (ORNL) and Los Alamos National Laboratory (LANL). For example, the team has prepared over 40 targets for LANL experiments at the Los Alamos Neutron Science Center (LANSCE). The stability of actinide targets also was tested with neutron irradiation at LANSCE. In-depth characterization of targets by high-resolution electron microscopy, diffraction methods, and alpha-particle spectroscopy before and after exposure to the neutron beams show no signs of degradation.

The grant provides for the education and training of the next-generation of scientists to exploit these new techniques and procedures. The project currently supports four graduate students from ND and Texas A&M Universities and six undergraduates from ND. The students have learned a wide range of experimental techniques related to actinide chemistry. These include the preparation of targets, characterization of materials by ion beam analysis and X-ray-based techniques, vibration spectroscopy, electron microscopy, and other methods. Two physics graduate students, Ashabari Mujumdar and Stefania Dede, participated in the neutron capture experiment at the LANSCE. Jordan Roach, a chemistry graduate student, has received a Glenn T. Seaborg fellowship and spent last summer at LANL working with Dr. Aiping Chen at the Center for Integrated Nanotechnology. Stefania Dede also had an internship at the LANL. She worked with Dr. Bredeweg and Dr. Rusev to analyze data from a neutron capture/fission experiment performed in June 2021 using the Detector for Advanced Neutron Capture Experiments (DANCE) detector array at LANSCE. Graduate students present their research results at multiple national and international conferences. They individually have received multiple postdoctoral position offers from both US and European national laboratories as a result of their talks.

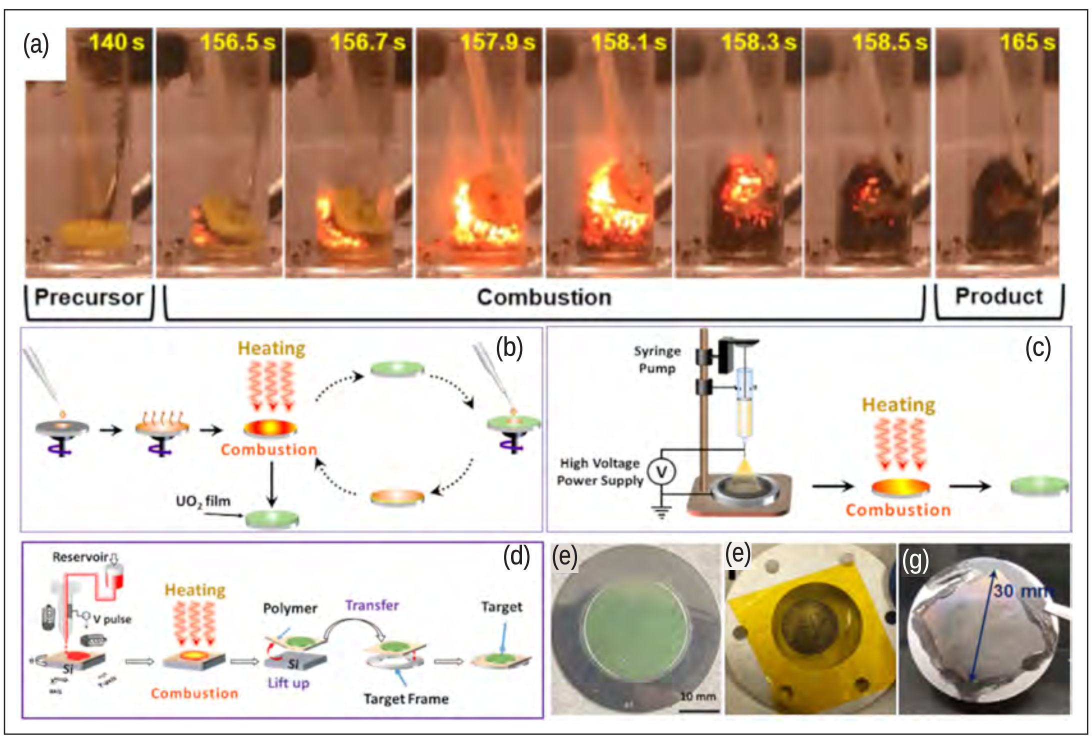
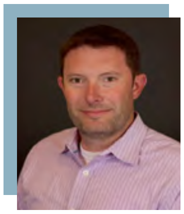


Figure 1. (a) Video recording for solution combustion synthesis (SCS) of uranium dioxide (UO_2) nanoscale materials and a schematic representation of actinide oxide film deposition by spin-coating-assisted-SCS. (b) Spray-assisted-SCS (c) Inkjet printing-assisted-SCS (d) Method with UO_2 targets deposited on aluminum (e) Kapton (f) and carbon (G) backings

Jason Jeffries, Lawrence Livermore National Laboratory (jeffries4@llnl.gov) ✦ **Years at LLNL:** 2007-Present
Degree: PhD, Condensed Matter Physics ✦ **SSAA:** 2003-2007, University of California, San Diego



I am a Senior Scientist in the Physics Division within the Physical and Life Sciences Directorate at Lawrence Livermore National Laboratory (LLNL). I currently serve as a Certification Lead for a product realization team and a Principal Investigator for a program within the laboratory's Additive Manufacturing Development portfolio. As a Certification Lead, I manage a broad swath of experiments and experimenters aimed at confirming or measuring materials properties and responses under extreme conditions. As a Principal Investigator, I direct an interdisciplinary group of scientists and engineers to enable new, agile manufacturing methods. These roles are somewhat disparate from a technical perspective, which just highlights the wealth of exciting research and development that occurs at LLNL in support of our myriad national security missions.

My first exposure to the Stewardship Science Academic Alliance (SSAA) came while I was pursuing my PhD research at University of California, San Diego with Prof. Brian Maple. During this time, we were funded by the SSAA to expand the high-pressure experimental capabilities to study f-electron physics under extreme conditions. At the crux of this research was integrating diamond anvil cells (DAC) into the extant low-temperature research equipment. I engaged with researchers at LLNL working on new, designer diamond anvils, small diamonds with embedded electrical circuits that enabled electrical measurements within the high-pressure chamber of the DAC. I traveled to LLNL several times to learn about DAC techniques, including many of the experimental tricks that researchers employed. These trips not only educated me, but they also spurred additional collaborations between the research group at LLNL and Prof. Maple's group. This collaboration resulted in a broad examination of magnetism under pressure in the Au-V system using multiple high-pressure platforms.

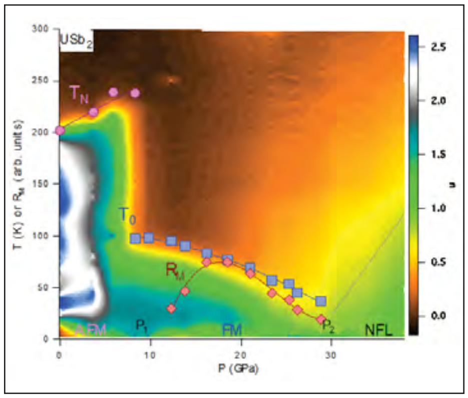


Figure 1. P-T phase diagram for the actinide magnet USb_2 under pressure showing the abrupt destruction of antiferromagnetism in favor of a ferromagnetic ground state just below 10 GPa. This abrupt change in the magnetic ground state is driven by a phase transition from a tetragonal to an orthorhombic structure. There is a smooth change in f-electron occupancy through this structural transition according to RXES data, suggesting that the magnetism is linked to the structure and not an underlying rearrangement of the electronic configuration. As the ferromagnetism is suppressed with pressure, a T-linear scattering emerges reminiscent of heavy-fermion materials driven toward a critical point [Jeffries, et al., Phys. Rev. B 93, 184406 (2016); Brubaker, et al., Phys. Rev. B 101, 085123 (2020).]

During my last year of graduate school, I attended one of the SSAA symposia and met Dr. Kerri Blobaum, who was looking for a postdoctoral researcher to join her project to look at phase stability in the Pu-Ga system. I joined LLNL as a postdoc, and I began working on plutonium research: phase stability, He bubble ingrowth, aging. While at LLNL, I also had the opportunity to continue my collaborations with the DAC group, where I learned about synchrotron techniques and married those with the electrical transport studies that I had executed as a graduate student. As I worked through these different research areas, I found that there were gaps in sample availability to really be able to answer the questions that we wanted to answer. So, I took a page out of Prof. Maple's laboratory and established a sample-preparation laboratory to produce tailored materials for small-scale experiments, and we used these samples to examine high-pressure properties of actinide compounds at the synchrotron. As I learned more about synchrotron capabilities, I was drawn back to some of the open questions in plutonium aging, particularly the aggregation of helium bubbles as the material ages. I leveraged my synchrotron experience to measure the bulk He bubble distribution in aged Pu using small-angle, X-ray scattering.

Figure 2. Quartz-tube sealing is a capability key to a variety of sample synthesis efforts supporting LLNL missions ranging from basic science to forensics to global security.

With the benefit of hindsight, I can see how my path unfolded from an SSAA-supported graduate student to an active researcher contributing to our national security missions. I never would have predicted this path. It is a testament to the SSAA program and its leadership that it is so effective at broadening its funding base to seed myriad foundational skills needed to advance our NNSA missions. SSAA support allowed me to explore the intersection of disciplines in my PhD work; and, while I didn't know it at the time, that fringe, that peripheral boundary is and always has been a fruitful area to explore.

Carolyn Kuranz, University of Michigan (ckuranz@umich.edu) ✦ **Years at UM:** 2009-Present
Degree: PhD, Applied Physics ✦ **SSAA:** 2002-2004, 2005-2009 University of Michigan

I am the Director of the Center for Laboratory Astrophysics (CLA) at the University of Michigan. I was first introduced to plasma physics in 1999, when I was a summer intern at Los Alamos National Laboratory (LANL). Overall, I was fascinated by the broad range of science that was being conducted at the laboratory, and I spent many afternoons in the library reading journals and learning new things. I spent several summers at LANL, until I finished my undergraduate degree in Physics from Bryn Mawr College in 2002. In one instance, I worked with Dr. Nels Hoffman using RAGE to model strong shock waves in materials. I was fascinated by the extreme states of matter in the high energy density (HED) regime. This directed me to graduate school at the University of Michigan in the Applied Physics program working with Professor Paul Drake and funded by the National Nuclear Security Administration (NNSA) Stewardship Science Academic Alliances (SSAA) Program. I did most of my PhD research at the Omega Laser Facility studying blast-wave drive, Rayleigh-Taylor instability relevant to core-collapse supernovae. On experiments, I worked closely with Drs. Harry Robey and Brent Blue at Lawrence Livermore National Laboratory and Dr. John Foster at the Atomic Weapons Establishment. In addition to creating blast-wave-driven instabilities, we were developing point-projection radiography to create high-resolution images of evolving instability growth. At the time, this presented several challenges but has gone on to be a commonly used imaging technique.

I finished my PhD in 2009 and became an Assistant Research Scientist at the University of Michigan funded by the NNSA Predictive Science Academic Alliance Program (PSAAP). This work was led by Professor Drake in collaboration with Professors Marv Adams and Jim Morel at Texas A&M University. Our goal was to develop a radiation hydrodynamics code with predictive capabilities and quantify the uncertainty in radiative shock experiments. I led the experimental efforts at the Omega Laser Facility and National Ignition Facility and worked to quantify the experimental uncertainty, which was part of our uncertainty quantification model.

In 2019, Professor Drake and I were awarded an SSAA Center of Excellence, the Center for Laboratory Astrophysics (CLA). The goal of CLA is to study fundamental HED science with relevance to astrophysics and the NNSA stockpile stewardship mission. I took over as Center Director in 2019 and joined the Nuclear Engineering and Radiological Sciences Department at the University of Michigan as an Associate Professor. I am continuing to explore systems that I first learned about as an undergraduate intern at LANL, and I continue to collaborate with the NNSA laboratories on my research. My students are largely funded by the SSAA programs and lead HED experiments at the Omega Laser Facility, the Z machine, and the National Ignition Facility and use radiation and magneto-hydrodynamics codes to simulate them. Our efforts increase our fundamental knowledge of these complex systems.

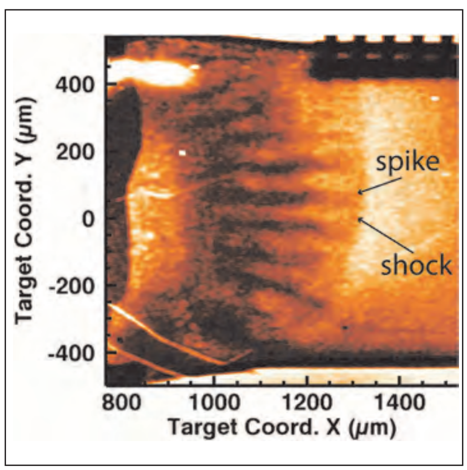


Figure 1. An X-ray radiographic image of an experiment that used a three-dimensional, single-mode perturbation as the initial condition. This radiograph was imaged 21 ns after the initial laser pulse began. Labels indicate the position of the shock and a spike extending to the shock front. From Kuranz, Physics Of Plasmas 17, 052709 (2010).

Through NNSA's Academic Programs, I've gone from being an intern at LANL, supported by both SSAA and PSAAP, to a Principal Investigator for a SSAA Center of Excellence mentoring the next generation of scientists to work at NNSA Laboratories. The NNSA Academic Programs are an excellent way to study extreme states of matter using state-of-the-art experimental and computational tools and interacting with NNSA scientists.

Through NNSA's Academic Programs, I've gone from being an intern at LANL, supported by both SSAA and PSAAP, to a Principal Investigator for a SSAA Center of Excellence mentoring the next generation of scientists to work at NNSA Laboratories. The NNSA Academic Programs are an excellent way to study extreme states of matter using state-of-the-art experimental and computational tools and interacting with NNSA scientists.

Zachary Matheson, National Nuclear Security Administration ✦ **Years at NNSA:** 2020-Present
Degrees: Dual PhD, Nuclear Physics; Computational Math, Science, and Engineering ✦ **SSAA:** 2014-2019 Michigan State University

I spent my time as a PhD student working with Witek Nazarewicz on furthering theoretical studies of nuclear fission in exotic regions of the nuclear chart. My connections with the Stewardship Science Academic Alliances (SSAA) program enabled me to perform calculations on Lawrence Livermore National Laboratory's (LLNL's) world-class supercomputers, to travel, to present my work at academic conferences, and to tour National Nuclear Security Administration (NNSA) science facilities (such as the National Ignition Facility (NIF) and the Z Machine). A highlight of my graduate student career was flying to Italy to give a talk about the element oganesson at a conference organized by Yuri Oganessian himself!

After graduating, I wanted to try my hand at science policy and oversight, so I applied and was accepted into the NNSA Graduate Fellowship Program. I worked for a year in the Office of Advanced Simulation and Computing, where I wrote white papers on hot topics such as deep learning and quantum computing. I attended a workshop on physics-informed machine learning and helped prepare a report to Congress on the use of artificial intelligence and machine learning within the NNSA. As a fellow, I was given special opportunities to attend trainings, conferences, and other professional development opportunities that broadened my horizons as a newly-minted PhD.

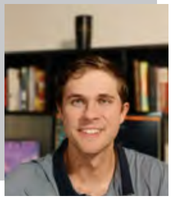
Post-fellowship, I joined the NNSA as a federal employee in the Office of Programming, Analysis, and Evaluation which provides decision support to program managers across NNSA. Whenever an NNSA program needs to develop a new science or production capability, my colleagues and I use modeling and simulation to forecast project risks and to estimate facility, personnel, and equipment needs. Then we use statistical and data science techniques to estimate things like project cost and schedule. We have a growing data set of past NNSA projects, and we use that data to create models we can use to predict future project costs. We deliver our results to higher-ups within NNSA through briefings and white papers, and we publish our methodologies within a wider community of decision support specialists across the world. In essence, my job is to know what's happening at the NNSA labs and sites well enough to provide defensible cost and schedule estimates to NNSA leaders and, ultimately, to Congress and the American people.

Figure 1. Matheson presents a cost estimating model developed using the method of quantile regression at the 2022 International Cost Estimating & Analysis Association's Professional Development & Training Workshop in Pittsburgh.

Even though I'm not doing basic nuclear physics research these days, a lot of my PhD skills have transferred to my current job. I still read and write papers and go to conferences. I write code and analyze data. I conduct studies, and I form and test hypotheses - same skills, different subject matter. And it's not just me – most of my colleagues were trained as physicists, chemists, and engineers.

There are other neat things about working where I do. Every morning I see the United States Capitol on my way to work, and every evening I run home along the National Mall. Though I am based in Washington DC, my colleagues and I travel regularly to NNSA's labs and sites across the country. But regardless of where we each live and work, the important thing is that the stuff you and I are doing is important work that matters to our elected representatives in government, our fellow Americans, and the rest of the world.

Sam Briney (sbriney@ufl.edu)
Degree in Progress: PhD, Mechanical Engineering, University of Florida ✦ Advisor: Dr. S. Balachandar ✦ SSAA: 2022-Present



Research Topic

Hydrodynamic Instabilities of Explosively-driven, Multiphase Fronts.

Research Responsibilities

My research involves computationally studying hydrodynamic instabilities of explosively-driven, multiphase fronts. Spherical and cylindrical blast waves in multiphase environments exhibit fingering instabilities which are not well understood presently despite their immense applicability in many national security contexts. My research aims to use the power of computational fluid dynamics to better understand the fundamental physics underlying these instabilities. My role in this project is to design and run Euler-Lagrange (EL) and particle-resolved simulations to help elucidate the details of the instability mechanisms underlying this observed, dispersed, multiphase phenomenon. The multiscale nature of the problem requires a multiscale solution approach, since the microscale flow results in emergent instabilities which only manifest at the mesoscale. Particle-resolved, microscale simulations provide a better understanding of the particle scale flow which, in turn, enable improved mesoscale EL simulations that can capture the important instability mechanisms of interest. These dispersed, multiphase flow simulations are massively parallel and utilize state of-the-art particle tracking algorithms and drag correlations, which our research group has developed over the past decade through a Predictive Science Academic Alliance Program (PSAAP) Center.

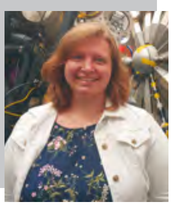
Benefits of SSAA

The Stewardship Science Academic Alliances (SSAA) program has benefited me considerably by providing the opportunity to run fascinating simulations, the results of which will provide insight into physics with implications for problems of national security interest. This is enabled by the SSAA's provision of extensive computing time without which conducting this research would be impossible. Additionally, the SSAA will allow me to attend conferences, enabling communication and collaboration with researchers in related fields.

What Students Considering SSAA Should Know

SSAA provides excellent opportunities to collaborate with Department of Energy (DOE) laboratories which, unequivocally, are some of the best research institutions in the world. Not only does working in collaboration with the great researchers at these labs give students insight into how to become better researchers, but it also enables them to network with those who can provide substantial post-graduation employment opportunities and internships.

Heather Garland (hig12@physics.rutgers.edu)
Degree in Progress: PhD, Physics and Astronomy, Rutgers University ✦ Advisor: Prof. Jolie A. Cizewski ✦ SSAA: 2016-Present



Research Topic

Towards Confirmation of the (d,pγ) Reaction as a Surrogate Reaction for (n,γ) in Inverse Kinematics with ^{95}Mo beams and GODDESS

Research Responsibilities

One diagnostic of nuclear device performance was to measure the yields of long-lived daughters of radioactive fragments following the fission of uranium and plutonium. The prompt fission fragments can be created or destroyed by neutron-induced reactions before they decay. One of these reactions is neutron capture. Therefore understanding (n,γ) reaction rates on fission fragments is important for stewardship science. Because prompt fission fragments are very short lived, indirect experimental methods are required to deduce (n,γ) reaction rates. One such indirect method is the Surrogate Reaction Method. The neutron transfer (d,p) reaction has been validated as a surrogate reaction for the (n,γ) reaction with beams of deuterons on a ^{95}Mo target (normal kinematics). In addition, the (d,p) reaction with beams of heavy nuclei (inverse kinematics) also needs to be validated. By impinging ^{95}Mo beams on C_2D_4 thin film targets, the (d,pγ) reaction was measured using GODDESS (Gammasphere ORRUBA Dual Detectors for Experimental Structure Studies). I am leading the selected reaction monitoring analysis of the data set obtained from the ^{95}Mo(d,pγ)^{95}Mo inverse kinematics experiment. I also have been active in the maintenance and implementation of the ORRUBA array.

Benefits of SSAA

A plethora of the incredible experiences throughout my career have occurred directly because of the support I receive from the Stewardship Science Academic Alliances (SSAA). As an undergraduate in 2016, the SSAA afforded me my first opportunity to work at a national laboratory, Oak Ridge National Laboratory (ORNL), with full time research scientists developing novel offline analysis routines. Encouraged by the cutting-edge science and support afforded to me from my collaboration with the SSAA, I chose to pursue a PhD in Nuclear Physics. The impact of the SSAA on my graduate career is immeasurable, as I have visited some amazing facilities, been on the forefront of science through experimentation, and networked with the leading physicists in my field.

What Students Considering SSAA Should Know

Expect the extraordinary. While in collaboration with the SSAA, I have participated in workshops and experiments at ORNL, Los Alamos National Laboratory, Lawrence Livermore National Laboratory, Lawrence Berkeley National Laboratory, the National Superconducting Cyclotron Laboratory, the Facility for Rare Isotope Beams, and Argonne National Laboratory. I have received so much more hands-on experience, because I work with the SSAA. As I finish my doctoral studies while in residency at ORNL, I cannot help but be excited for my future in Nuclear Physics.

Jes Koros (jkoros@nd.edu)
Degree in Progress: PhD, Nuclear Physics, University of Notre Dame ✦ Advisor: Prof. Anna Simon-Robertson ✦ SSAA: 2020-Present

Research Topic

Constraining Neutron Capture Cross Sections with Surrogate Reaction Measurements

Research Responsibilities

Our understanding and models of nuclear processes are informed by nuclear data, including cross sections and reaction rates. When the reactions of interest cannot be performed directly in the lab, there are cases where measurements of surrogate reactions may be used to constrain these quantities. My research involves constraining neutron capture cross sections with surrogate reaction measurements. I'm involved with preparing and performing experiments as well as the analysis of the experimental data. This involves operating detector and accelerator systems, developing analysis programs, and performing calculations to incorporate experimental results into theoretical models.

Benefits of SSAA

The collaborations enabled by the Center for Excellence in Nuclear Training and University-Based Research (CENTAUR) have been integral to my thesis work. As a CENTAUR student, I have had several opportunities to visit the national laboratories and learn about their career paths. These connections have led to opportunities to work with laboratory scientists, including during an internship at Lawrence Livermore National Laboratory (LLNL) in Summer 2022.

Figure 1. University of Notre Dame PhD student, Jes Koros, at the Hyperion detector array at Texas A&M University's Cyclotron Institute.

New Contacts, New Opportunities

My experimental work is enabled by the collaboration between the University of Notre Dame, Texas A&M University (TAMU), and LLNL through CENTAUR. My thesis experiment was performed at TAMU's Cyclotron Institute with LLNL's Hyperion array. This campaign was performed in conjunction with an LLNL experiment, providing me the opportunity to work directly with researchers from both LLNL and TAMU.

I also had the opportunity to spend a summer at LLNL through the Seaborg Internship. This gave me a great look at the life of a lab scientist and created connections that are helpful in both my immediate research and future career. While at LLNL, I was able to further my data analysis by working with experimentalists and theorists to gain valuable insight from their experience. Additionally, I gained a broader understanding of the lab's work as a whole through exposure to more interdisciplinary seminars and collaborations.

Tanja Kovacevic (tanya_kovacevic@berkeley.edu)
Degree in Progress: PhD, Earth and Planetary Science, University of California, Berkeley ✦ Advisor: Burkhard Militzer ✦ SSAA: 2020-Present

Research Topic

Condensed Matter Physics/Astrophysics

Research Responsibilities

My research focuses on performing *ab initio* molecular dynamics (AIMD) to predict the thermodynamic material properties at extreme conditions. In a recent collaboration with Professor Sarah T. Stewart (UC Davis) and in a subsequent publication, we investigated the miscibility (homogeneous mixing) of $MgSiO_3$ (rock) and H_2O (ice) at conditions relevant to the interiors of water worlds. We investigated whether the rock-ice boundary layers of these exoplanets remain well separated or if the rock and ice become miscible at the pressure-temperature conditions of the boundary. Our work found that many water-rich exoplanets likely have mechanically-mixed layers as they form.

Benefits of SSAA

My access to the supercomputer cluster at Lawrence Livermore National Laboratory (LLNL) played a crucial role in allowing me to efficiently finish my calculations. The yearly Stewardship Science Academic Alliance (SSAA) symposiums offer me a chance to share my research, to network with colleagues, and to learn how I can transfer the techniques I have learned to other fields of research at national laboratories around the Unites States.

When I first began at UC Berkeley, I was a recent graduate with a BS in chemistry, and making the switch into condensed matter physics meant I had plenty of learning ahead of me. However, the various seminars given throughout the year by the Chicago/Department of Energy Alliance Center and the Center for Matters under Extreme Conditions helped me build the high energy density physics fundamentals necessary for my successful transition into this new field.

Through the training I am receiving, with the support of the SSAA, I am becoming the scientist I always dreamed as a young girl that I could become. On a personal note, as a first-generation college student and refugee the SSAA has given me invaluable tools for navigating my career after I finish my PhD studies.

Lauren Poole (lpoole@ucsb.edu)

Degree in Progress: PhD, Materials Science, University of California, Santa Barbara ✦ **Advisor:** Prof. Frank Zok ✦ **SSAA:** 2019-Present

Research Topic

High-Strain-Rate Mechanical Behavior of Multiphase Metals

Research Responsibilities

I am a student in the multi-university, Stewardship Science Academic Alliances (SSAA) Center for Research Excellence on Dynamically Deformed Solids (CREDDS). The overarching goal of CREDDS is to develop complex, multiphase metals and to understand their response under quasi-static and dynamic loading conditions. My own research aims to understand the role of strain rate, phase topology, and constituent phase properties on mechanical response with a specific focus on composites with co-continuous phase distributions. I am the primary user of the CREDDS split-Hopkinson pressure bar system, meaning I design and run my own experiments and assist collaborators in testing the materials they develop. I also perform mechanical tests at the University of California Santa Barbara (UCSB) and at Los Alamos National Laboratory (LANL), characterize my materials in two and three dimensions, and run finite element simulations.

Benefits of SSAA

The SSAA program and CREDDS afford the opportunity to work in a center that provides structured opportunities to collaborate with talented students and professors across several universities. Through these collaborations, I get access to specialized equipment (such as the split-Hopkinson pressure bar, gas guns, ultra-high speed imaging capabilities, the UCSB TriBeam, and computing facilities) that allows me to conduct unique and rigorous work combining experiments and simulations. I am exposed to the breadth of exciting research at National Nuclear Security Administration (NNSA) laboratories and get to explore potential career opportunities through SSAA events, conferences, and collaborations.

National Laboratory Experience

I spent the Spring 2022 academic quarter at LANL working with Dr. Saryu Fensin on the Dynamic and Quasi-Static Loading Team. As someone interested in working at the lab, I enjoyed getting to make connections, work with experts in the field, and experience how research is carried out in a lab setting. At LANL, we conducted flyer plate impact experiments using a gas gun to probe material response at very high strain rates (10^4 s^{-1} and above). This strain rate regime is of particular interest because metals begin to exhibit a heightened rate sensitivity and fail via spall. Our research aims to elucidate the microstructural origins of spall which become more difficult to predict when you introduce a second phase. I benefited from collaborating with LANL scientists, because achieving very high strain rate loading conditions requires specialized equipment rarely found at universities.

Jordan Roach (jroach4@.nd.edu)

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

Research Topic

Combustion Synthesis of Actinide Oxides

Research Responsibilities

My research investigates the rapid production of actinide oxides via combustion synthesis. These reactions take advantage of the highly exothermic interaction between a metal nitrate and organic reductants (fuel) to produce metal oxides. This work is applied by our group to the making of actinide thin films for use as targets in nuclear physics research. Such applications have led to the collaborative production of targets for research at Los Alamos National Laboratory (LANL). The use of a combustion synthesis method provides a rapid, energy-efficient process for producing bulk nanoscale and thin-film oxide materials. Our work with uranium oxide has shown that by controlling several factors, individual oxide phases can be produced selectively. Investigations into the mechanism of combustion reveal active participation by intermediate actinide complexes. Current research into the participation of these compounds aims to fine tune these reactions for the synthesis of metastable oxide phases.

Benefits of SSAA

Funding from the Stewardship Science Academic Alliances (SSAA) program has helped grow a close collaborative relationship between the Nuclear Science Laboratory and Actinide Research Labs at the University of Notre Dame. As a chemist, I have enjoyed working closely with my physicist counterparts in learning more about each other's fields and using our respective strengths to bolster our research. In addition to creating a strong internal collaboration, SSAA funding has allowed for a number of external collaborations both at the national labs and at other academic institutions. Funding for travel has allowed for me and other graduate students to attend a variety of conferences to not only share our work but to greatly expand our professional network in our areas of research.

National Laboratory Experience

This past summer I was fortunate enough to spend three months as a Seaborg Institute Graduate Research Assistant in the Center for Integrated Nanotechnology at LANL. I found this time to be a fantastic experience in learning about different opportunities at LANL. The internship gave me a wonderful insight into the general logistics of conducting actinide research and working at a national lab. This experience encouraged me in wanting to pursue a position at a national lab to continue actinide research. This is not only because of the numerous opportunities but also the capabilities of the national lab system compared to traditional research at universities.

High Energy Density Laboratory Plasmas Program

Particle Heating by High-Mach-Number, Collisionless Shocks in Magnetized Laboratory Plasmas | Princeton University

PI: Dr. Derek Schaeffer (dereks@princeton.edu)

As a fundamental process for converting kinetic energy to thermal energy, collisionless shocks are ubiquitous throughout the universe from planetary bow shocks to supernova remnants. Whereas they have been studied for decades by spacecraft and numerical simulations, there remains a key open question of how energy is partitioned between particles across a shock. The goal of this project is to study this shock heating process and dependence on shock structure in well-controlled and well-diagnosed laboratory experiments. This will help benchmark simulations that bridge the gap between laboratory and astrophysical systems. One postdoctoral fellow and one graduate student will help design and execute experiments and will perform data analysis and numerical simulations.

Shocks, especially fast or high-Mach-number shocks, are a key component of astrophysical plasmas and are known to energize particles to some of the highest energies observed in the cosmos. In collisionless plasmas, these shocks are mediated by electromagnetic fields instead of particle collisions and act to slow down supersonic flows to subsonic speeds by heating particles. A critical outstanding problem in shock physics is how the energy of the supersonic flow is split between heating electrons and ions. Collisionless shocks have been studied by spacecraft for decades, but due to limited spacecraft trajectories and highly variable systems, these observations have not been able to reveal the mechanisms by which particles are shock heated. Laboratory experiments can help address this problem.

To create collisionless shocks in the lab, a supersonic flow needs to expand into a background plasma embedded in a strong magnetic field. This can be accomplished at the Omega Laser Facility, part of the Laboratory for Laser Energetics at the University of Rochester (Figure 1a). The experiments start by pulsing a set of copper coils to generate a strong magnetic field. A laser then hits a target to create a background plasma that fills the volume between the coils. High-energy lasers then irritate another target to create a fast moving piston plasma. The piston acts to sweep up the background plasma and magnetic flux like a snowplow, accelerating it to supersonic speeds to drive a shock.

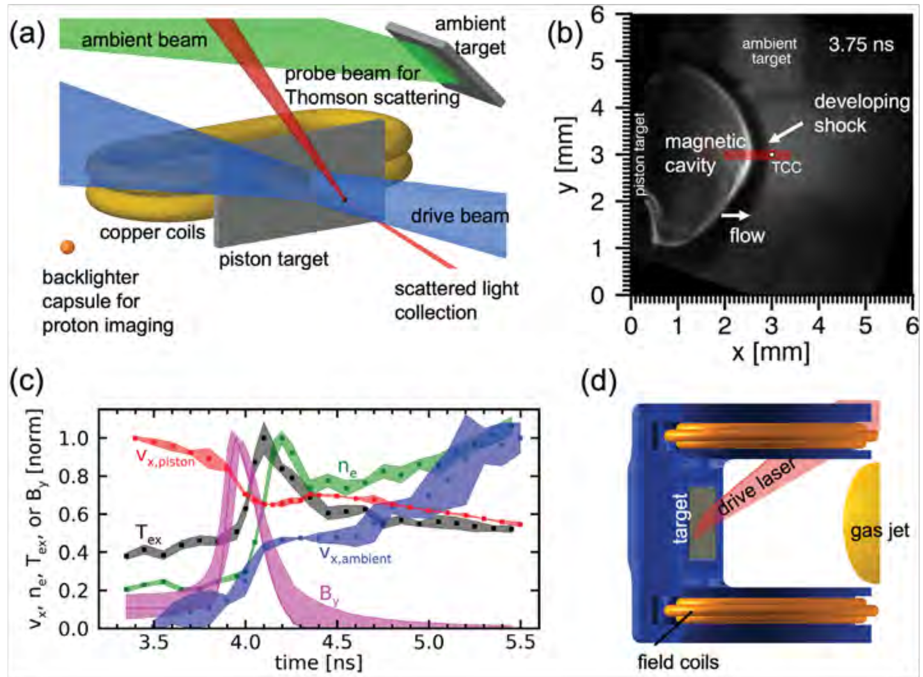


Figure 1. (a) Schematic of experimental setup on OMEGA 60. (b) Proton image showing magnetic field structure associated with developing shock. (c) Profiles of density (green), temperature (gray), magnetic field (purple), ambient ion flow speed (blue), and piston ion flow speed (red) measured with Thomson scattering and proton imaging. (d) Schematic for new experimental platform for larger system

The resulting magnetic field structures are diagnosed with proton imaging. Laser beams irradiate a small capsule filled with DHe^3 gas placed outside the copper coils which generates a proton beam as a fusion by-product. The protons travel through the shock and get deflected before traveling to a detector. By analyzing the proton patterns on the detector, the structure of the magnetic field can be deduced Figure 1b). Plasma parameters, including temperature, are diagnosed with optical Thomson scattering. A probe laser is directed through the shock region, where some light is scattered by the plasma. The scattered light is collected and passed through spectrometers and onto a charge coupled device (CCD) detector. By fitting the resulting spectrum with a model of the scattered power, plasma parameters like density, temperature, and flow speed can be extracted (Figure 1c).

Previous experiments with this platform have demonstrated high-Mach-number, collisionless shock formation[1] and the ability to measure particle heating using Thomson scattering in a developing shock.[2] A key limitation of those experiments was that the shock could not evolve long enough to fully separate from the piston, which is required to study shock heating. To address these limitations, a new experimental platform has been developed that utilizes a larger set of coils and a gas jet to create an ambient plasma (Figure 1d). This new platform allows the magnetic fields and ambient plasma to be more uniform and the volume of magnetized ambient plasma to be significantly larger. As a result, upcoming experiments will extend previous results to longer timescales where particle heating can be measured in fully formed shocks.

References

[1]Schaeffer, et al., Physical Review Letters 119, 025001 (2017).

[2]Schaeffer, et al., Physical Review Letters 122, 245001 (2019).

Electron-Ion Equilibration in Dense and Quantum Plasmas | University of Nevada, Reno

PI: Dr. T.G. White (tgwhite@unr.edu)

Funded through the High Energy Density Laboratory Plasmas (HEDLP) program, this project, led by researchers at the University of Nevada, Reno, aims to study the process of electron-ion equilibration in warm dense matter. This National Nuclear Security Administration (NNSA) grant supports a postdoctoral scholar, a graduate student, and two undergraduate students.

When a high-intensity laser is incident on a solid target, the material is brought into a state far from equilibrium. The preferential and rapid heating of one subsystem over the other creates highly-coupled, cold ions immersed in a hot, partially-degenerate, electron sea. These non-equilibrium, high energy density plasmas are a precursor to warm dense matter—states routinely created during laser micromachining and inertial confinement fusion (ICF) experiments. In the laboratory, these transient states serve as a testbed, where quantum mechanical theories of electron-ion interactions, nuclei dynamics, and phase transitions can be validated.

The mechanism and relevant timescales of the electron-ion equilibration process are not well understood, and current theoretical approaches give results that differ by over an order of magnitude. Furthermore, experimental measurements in this regime are difficult. Despite being a fundamental thermodynamic quantity, the ion temperature had never been directly measured in a dense plasma.

The team has developed an X-ray scattering platform for free-electron lasers (FELs) with a resolution capable of measuring the ion temperature in a dense plasma. By backscattering a highly monochromatic source of X-rays off the plasma, they are able to measure the width of the quasi-elastic Rayleigh peak. In this geometry, the width of the peak is essentially governed by Doppler broadening which directly measures the ions' velocity distribution. For non-degenerate ions with a Maxwellian distribution, this corresponds to a model-independent temperature measurement.

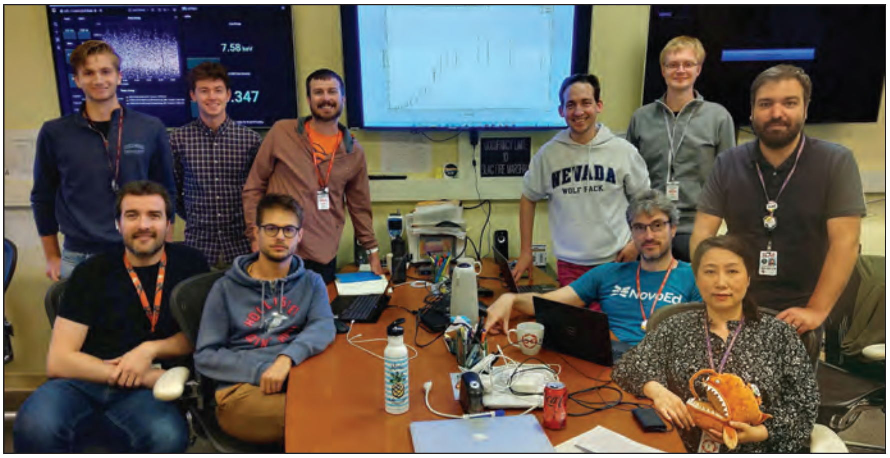


Figure 1. Back row: Carson Convery (SLAC), Ben Armentrout (SLAC), Daniel Haden (UNR), Thomas White (UNR), Lennart Wollenweber (EuXFEL), and Dimitri Khaghani (SLAC). Front row: Eric Galtier (SLAC), Adrien Descamps (SLAC), Bob Nagler (SLAC), and Hae Ja Lee (SLAC).

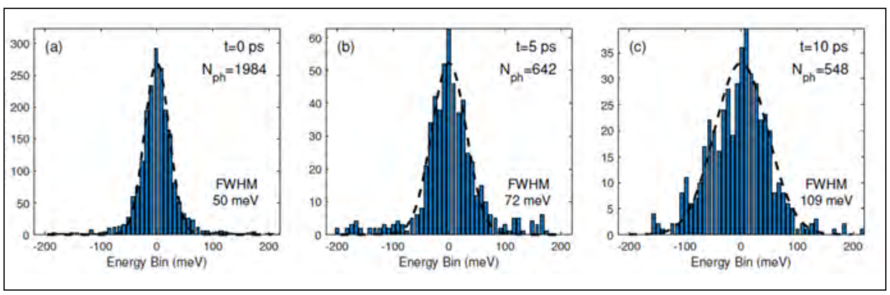


Figure 2. Preliminary data on laser irradiated gold. The efficacy of the method is demonstrated in high-resolution spectra taken at (a) 0 ps, (b) 5 ps, and (c) 10 ps after laser irradiation. The spectra show clear broadening of the quasi-elastic Rayleigh peak. This data was taken from 50 nm gold samples irradiated at an intensity of ~ 10^{14} W/cm^2. We recorded an average of two photons per shot, with the total number detected given for each spectrum.

In May 2022, the team (shown in Figure 1) performed an experiment at the Linac Coherent Light Source (LCLS) where they unambiguously measured electron-ion energy equilibration in gold and silver foils just 50 nm thick. A short pulse Ti:Sapphire laser focused to a 100 µm spot is used to initiate the energy cascade between electron and ion populations. Only modest laser intensities of 10^{13}–10^{14} W/cm^2 are needed to heat these targets to electronvolt temperatures, and ballistic transport of fast electrons ensures uniform heating. The temporal evolution of the ion temperature is tracked with sub-picosecond resolution with the X-ray beam. Time delays up to a few tens of picoseconds, which is before any hydrodynamic expansion occurs, ensures the measurement will take place at a known (solid) density.

In these novel experiments, the difficulty in measuring the ion temperature can be attributed to the large ion mass. The broadening of the quasi-elastic Rayleigh peak is small compared to that of the electrons. The required high resolution is achieved by taking the seeded beam of LCLS, which already has a reduced bandwidth (~1 eV) compared to the SASE mode (~10 eV), and further reducing the bandwidth by passing it through a 4-pass Si (533) monochromator. The scattered X-rays are collected on diced crystal analyzers positioned at differing angles. At an incident energy of 7.5 keV, the entire setup allows for measurements over a >500 meV energy range and with an energy resolution of ~50 meV.

Figure 2 shows preliminary data from the experiment demonstrating the success of the technique. The width of the quasi-elastic Rayleigh feature is clearly broadened at delays of 5 ps and 10 ps after the optical laser pulse. Corresponding to an increase in the ion temperature of ~10,000 K over the course of 10 ps.

Forrest Doss, Los Alamos National Laboratory (fdoss@lanl.gov) ✦ Years at LANL: 2011-Present
Degree: PhD, Applied Physics, University of Michigan ✦ HEDLP: 2010-2011; PSAAP II: 2008-2010

During my time as a graduate student at Michigan, my work was supported by one of the first rounds of the Predictive Science Academic Alliance Program (PSAAP) centers, one of the first years of the Department of Energy (DOE) Stewardship Science Graduate Fellowship (SSGF) fellowships, and by the joint program in High Energy Density Laboratory Plasmas (HEDLP). My work during graduate school focused on high energy density experiments on radiative shocks, shock waves for which the speed and temperature are turned up so high that the feedback from their own heat significantly reshapes them. The experiments themselves were carried out at the Omega Laser Facility at the Laboratory for Laser Energetics (LLE) in Rochester, NY, but my research included many opportunities to visit and engage with DOE's national laboratories.

As a graduate student, an extended stay at Lawrence Livermore National Laboratory (LLNL) let me temporarily abandon my other responsibilities so that I could learn to run the lab's multiphysics HYDRA code. The DOE codes are large and complex, and learning to use them effectively is a skill. Returning to Michigan, I was able to put this to work modelling the laser-driven laboratory plasma experiments to which I returned, and I then was able to take those skills to my first staff job at Los Alamos National Laboratory (LANL).

At LANL, my focus has been on designing experiments to test the applicability of turbulence models in high energy density plasmas. LANL's home-grown turbulence models,[1] which are calibrated to traditional fluid experiments, are expected to be applicable to dense, hot plasmas, but this expectation needs to be assessed. Only if the model can reproduce simpler, dedicated, instability experiments can it be trusted in complex, integrated, fusion experiments driven on the same laser.[2]

Since 2018, I have been a guest of the Sandia National Laboratories' Pulsed Power Sciences Center, the home of the Z Machine. Unlike a laser, which drives targets into the plasma state with intense light, the Z machine is a so-called "pinch" facility that implodes the targets with extreme currents. This can be used to drive experiments that are different and complementary to the laser-driven instability experiments[3] and have been used to study the behavior of LANL's physics codes in yet another regime, further extending our confidence in our models. The design of all of these experiments has been made possible by the opportunities I was given by the NNSA academic programs all the way back to graduate school, including the opportunities to build relationships throughout the DOE national laboratories.

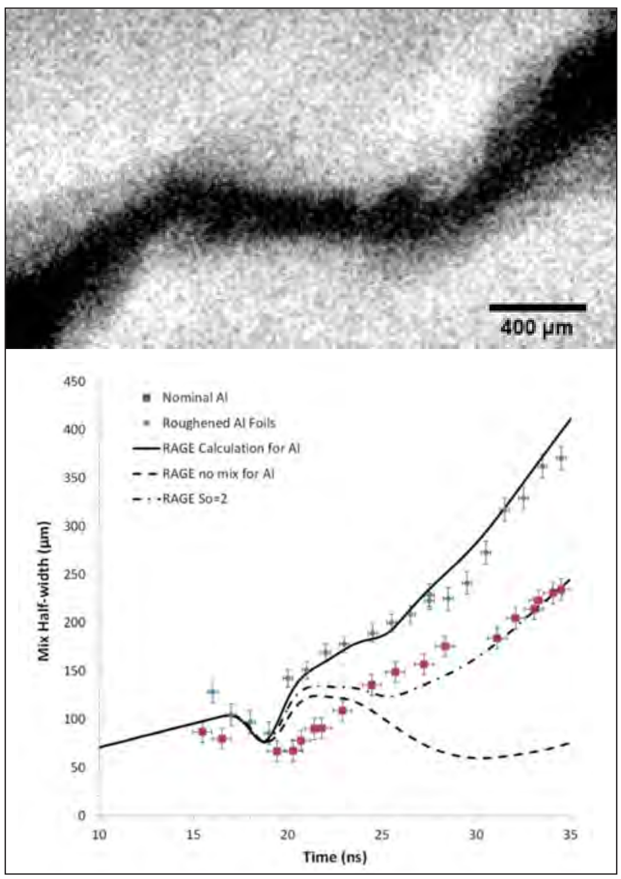


Figure 1. Above, this radiograph from NIF Experiment N141006 shows the creation of swirling vortices which can be studied by turbulent mixing model in LANL's multiphysics RAGE simulation code.[2] This has the same characteristics as classical turbulence experiments, but driven with flows over 100 km/s in speed, form their instability in only nanoseconds and reach deeply into the plasma regime. Below, data (points) and simulations (curves) of these experiments show the ability of the model to match the experimental settings as the instability evolves and how different settings for the model match different degrees of roughness.[4] The dashed curve shows the simulation without the mixing model, which cannot match the growth of data, showing how the model is essential for capturing turbulent mixing behavior.

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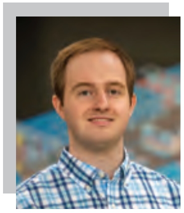
[2]Doss et al., "The Shock/Shear platform for planar radiation-hydrodynamics experiments on the National Ignition Facility", Phys. Plasmas 22, 056303 (2015).

[3]Knapp et al., "A novel, magnetically driven convergent Richtmyer–Meshkov platform" Phys. Plasmas 27, 092707 (2020)

[4]Flippo, et al., "Late-time mixing and turbulent behavior in high-energy-density shear experiments at high Atwood numbers" Phys. Plasmas 25, 056315 (2018).

Patrick Adrian (pjadrian@mit.edu)
Degree in Progress: PhD, Nuclear Science and Engineering, Massachusetts Institute of Technology ✦ Advisor: Dr. Johan Frenje
HEDLP: 2017-Present

Research Topic



Charged Particle Transport in High Energy Density Plasmas

Research Responsibilities

I am responsible for conducting my own experiments at the Omega Laser Facility. My experiments study charged particle transport in high energy density plasmas (HEDP). Charged particle transport is critical for understanding how mass, momentum, and energy are transported around HEDP. This transport is critical to model correctly in order to utilize HEDP for inertial fusion, stockpile stewardship, and laboratory astrophysics experiments. Part of my responsibilities is diagnostic development and analysis. I have worked extremely closely with scientists at Lawrence Livermore National Laboratory (LLNL) to utilize X-ray and nuclear diagnostics at both OMEGA and the National Ignition Facility.

Benefits of HEDLP

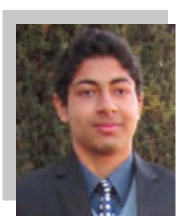
The experiments I conduct involve working with a large team of scientists and engineers from the University of Rochester in addition to other collaborating scientists at the national laboratories and other institutions. The HEDLP program has enabled these connections in my own research and have helped me to cultivate a network of scientists to work with collaboratively. This has significantly improved my own research by exposing me to a diverse set of opinions and methods held by many scientists in the field. It is this comingling of ideas from which I have benefitted the most.

New Contacts, New Opportunities

I spent two summers at LLNL and one summer before graduate school at Los Alamos National Laboratory. These experiences have solidified my interest in becoming a scientist at a national laboratory. During these summer internships I was able to help other scientists conduct research on a wide variety of topics from fast-ion stopping power to shock wave propagation. I was able to see the collaborative work environment of the national labs and how they tackle very large problems in the national interest. While doing so, I was able to learn and add new tools to my own scientific toolbelt. Each summer I learned new skills that I have incorporated into my own PhD thesis work. Overall, my experiences at the national labs has made me a better scientist and have stimulated my interest to continue working in the dynamic national lab environment.

Ahmed Elshafiey (ae389@cornell.edu)
Degree in Progress: PhD, Electrical Engineering, Cornell University ✦ Advisor: Dr. David Hammer ✦ HEDLP: 2017-Present

Research Topic



Time-resolved X-ray Spectroscopy on Hybrid X-pinches

Research Responsibilities

Understanding the formation of hotspots that are responsible for the X-ray bursts observed in X and Z-pinches is very difficult due to their temperature (>800eV), electron density (>10^{21}/cm^3), size (<1 μm), and duration (<1 ns). Radiative collapse is one of the proposed mechanisms for the formation of such hotspots. It is a runaway process in which radiation cools the plasma, assisting the magnetic field pressure in pinching it further, reducing its radius and increasing its density. Because radiation is proportional to the density squared, this process continues until the minimum radius is reached at which opacity effects or instabilities cause the explosion of the hotspot. Through the usage use of picosecond, time-resolved, X-ray cameras to study the K- and L-shell emission lines and radiation magnetohydrodynamics (RMHD) simulation codes, we have been able to study such hotspots and shine a light on other mechanisms that could be contributing to the formation of such spots. My research responsibilities varied from performing experiments and data analysis to designing and machining the loads and running simulations to understand the experimental results.

Benefits of HEDLP

The field of atomic spectroscopy in plasma physics is a very difficult field due to the background requirements, but attending conferences and symposiums, including those of the Stewardship Science Academic Programs, American Physical Society Division of Plasma Physics, and the International Conference on Plasma Physics, and networking with other scientists in the field is one of the important skills I have learned. I've been able to access a variety of simulation codes developed by Los Alamos National Laboratory (LANL) and Sandia National Laboratories without which I wouldn't have been able to analyze some of the experimental data obtained. I've worked closely with the Laboratory for Laser Energetics in some of the collisional radiative simulations that otherwise I wouldn't have been able to run on my own. In addition, I have been able to attend summer schools where I've met other students working on similar projects and exchanged ideas with them. Finally, networking was very useful when it came to applying for jobs, as I was able to land a postdoc opportunity at LANL starting in February 2023.

Facility Access and Community Development Programs

Facility Access Program

In 2022, the Facility Access Program supports travel for researchers who are granted shot time at the Omega Laser Facility. This provides hands-on research experience to academic and industrial researchers using the OMEGA and OMEGA EP lasers as tools for conducting basic research experiments. In 2023, travel support will also be offered to researchers who have been awarded time at NIF and other NNSA facilities. In the pursuit of fundamental science advances, the innovative development of diagnostics and platforms by user facility partners have often proven to benefit NNSA experimental needs.

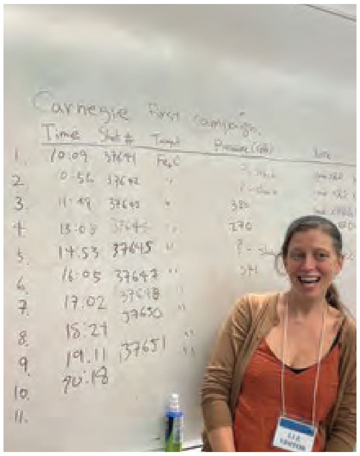
Community Development

Community Development supports specialized educational opportunities that both train and attract students to high energy density science. The High Energy Density Laboratory Plasmas program provides travel support for students to attend the High Energy Density Science summer school and various facility workshops. In 2022, 23 students were given travel support to attend the Z Fundamental Science Workshop in Albuquerque, New Mexico.

The Z Fundamental Science Workshop is a key aspect of the Z Fundamental Science Program. This Workshop, which has been held annually since 2010, consists of both Plenary and Breakout sessions. The Plenary sessions are meant for the external Z user community to hear about the Z accelerator facility status and future plans, receive an update on Z diagnostics capabilities, and for collaborative users to present the status of their research. The breakout sessions provide opportunities for current and prospective future collaborators to discuss research directions and ideas for new work on Z; many of these discussions are the genesis of Z Fundamental Science Proposals. The 13th Z Fundamental Science Workshop returned to an in-person format (the previous 2 Workshops were fully virtual) and was extremely successful, with 124 in-person attendees (56 external to Sandia) from 24 institutions and 2 countries, including 29 students and 13 post docs. Most of the student and post doc attendance was made possible through the generous support of the NNSA Academic Programs. This group was very engaged during the Workshop and many enthusiastically participated in a vibrant poster session. Student and post doc involvement in the Workshop is critical to growing the user base for Z and attracting the next generation of talent to the Pulsed Power Sciences Center at Sandia.

Dr. Marcus D. Knudson
Senior Scientist
Sandia National Laboratories

Carnegie postdoc Sota Takagi in OMEGA EP viewing gallery.



Carnegie scientist Sally Tracy in OMEGA EP control room.

Omega Laser Facility, Laboratory for Laser Energetics, University of Rochester

Predictive Science Academic Alliance Program III

CESMIX: Center for the Exascale Simulation of Material Interfaces in Extreme Environments | Massachusetts Institute of Technology

PI: Dr.Youssef Marzouk (ymarz@mit.edu)

The Center for Exascale Simulation of Materials in Extreme Environments (CESMIX) is a single-discipline PSAAP III center 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.

CESMIX's overarching goal is to predict the degradation of complex materials in extreme environments, from first principles. As an exemplar of this goal, the center focuses on materials exposed to ultra-high temperatures, extreme heat fluxes, and oxidative chemical environments on the leading edges of hypersonic vehicles. This setting is generally inaccessible to direct experimental observation, and predicting material properties in such environments is enormously difficult. CESMIX addresses this challenge by developing a comprehensive new multiscale materials simulation framework, bridging from multiple levels of electronic structure theory to classical molecular dynamics to continuum scales.

Molecular simulations of hafnium oxidation. We have performed our first end-to-end molecular simulations of Hf oxidation, which is a first simulation target on our roadmap towards more complicated materials. This process involved benchmarking density functional theory (DFT) functionals for hafnium-containing systems, automated generation of DFT data, training of machine learning interatomic potentials (including graph neural network potentials), molecular dynamics simulations with these potentials, and the development of an off-lattice kinetic Monte Carlo scheme for longer-time simulation (Figure 1). We have also developed a new "proper orthogonal descriptor" potential for molecular dynamics simulation, which derives a reduced set of invariant descriptors of atomic environments using reduced basis techniques, and shows substantial speedups over SNAP and Allegro potentials for the same level of accuracy.

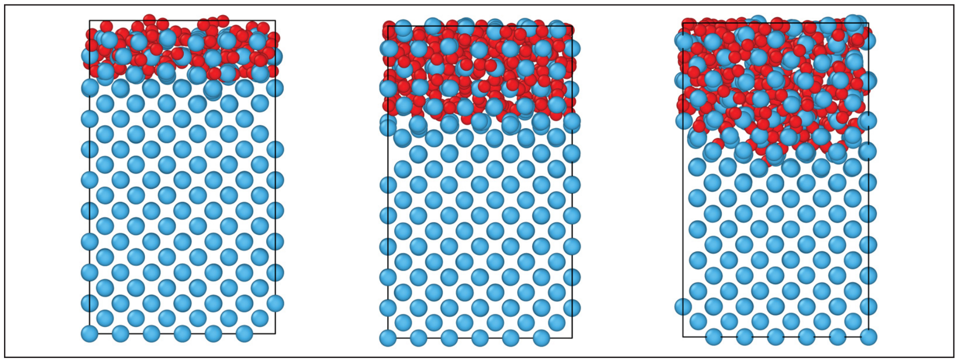


Figure 1. Off-lattice kinetic Monte Carlo simulations of hafnium oxidation.

Julia integration. A core aspect of CESMIX is the development of a Julia-based integrated molecular simulation ecosystem. This collection of software packages exploits core features of Julia, a high-level programming language, but emphasizes interfaces and abstractions that allow for inter-operability and composability of multiple density functional theory codes (e.g., QuantumESPRESSO and the Julia-native DFTK.jl), molecular dynamics simulators (e.g., LAMMPS and the Julia-native Molly.jl), and a variety of different interatomic potentials. Our workflow has advanced to the point where a user can seamlessly build and fit new interatomic potentials with relatively few lines of code, aided by composability and a common set of underlying abstractions and data structures.

UQ and active learning. We have advanced UQ and active learning methods for molecular modeling, with an emphasis on kernel-based methods. Specifically, we have devised probabilistic methods for selecting informative subsets of atomic configurations based on determinantal point processes (DPPs), using kernels based on descriptors of atomic environments. We have also devised kernelized active learning strategies, designed to create new atomic configurations that improve the diversity and coverage of training sets by modifying the underlying molecular dynamics. Another ongoing effort involves devising statistical techniques for assessing the errors in DFT predictions, based on multi-task modeling.

Parallel compiler technologies. An ongoing effort involves advancing compiler technologies for parallel performance and portability. Key thrusts this year include work on the Kitsune compiler toolchain, targeting GPUs, in collaboration with LANL. We have also begun integrating the Tiramisu domain-specific language (DSL), for dense and sparse computations, with the OpenCilk compiler. This effort lays the groundwork for using DSLs in molecular dynamics computations. Another ongoing CESMIX effort involves the pervasive use of differentiable programming. We are expanding the scope and capabilities of Enzyme, an automatic differentiation compiler plugin for the LLVM compiler framework. 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. Enzyme is used throughout CESMIX, and is being adopted by other PSAAP III centers as well.

Current 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, six postdoctoral associates, eight graduate students, two undergraduate researchers, and a research software engineer, plus several external collaborators.

Center for Exascale Monte Carlo Neutron Transport | Oregon State University

PI: Dr. Todd Palmer (todd.palmer@oregonstate.edu); Author: Dmitriy Anistratov, North Carolina State University

Elementary particles are everywhere. They surround us and influence the physical world. Some of these particles move freely, collide, and interact. Particles born in the Sun travel to the Earth, penetrate the atmosphere, and make weather. Other particles can be used to produce energy, treat diseases, and peer inside a human body. To use the innate talents of particles to design technologies, we need accurate models that describe the complicated and beautiful world of particles starting from their microscopic level up to our macroscopic scale. The Boltzmann equation describes the statistical properties of an ensemble of particles and predicts the evolution of the particle density function. The moments of this function connect the parts of the world at the different scales. We can use our fundamental knowledge about the lives of particles and the Boltzmann equation to model the interaction of particles with matter, based on first principles, in a variety of physical systems, including nuclear reactors, plasmas, high energy density physics, etc.

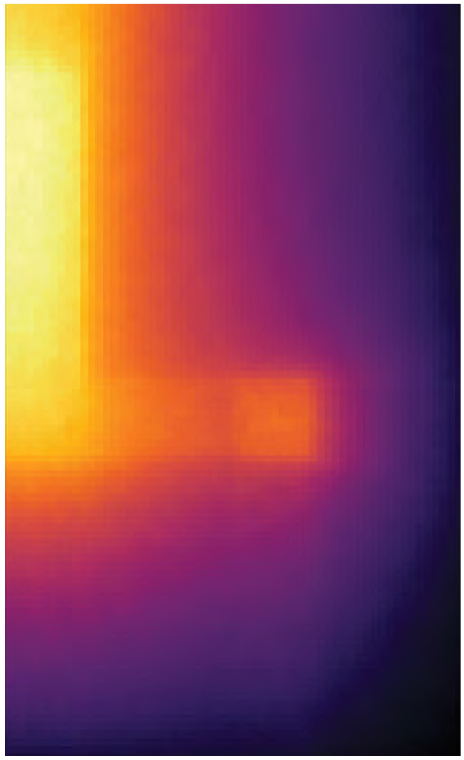


Figure 1. Neutron flux in time-dependent Kobayashi benchmark problem calculated in MC/DC.

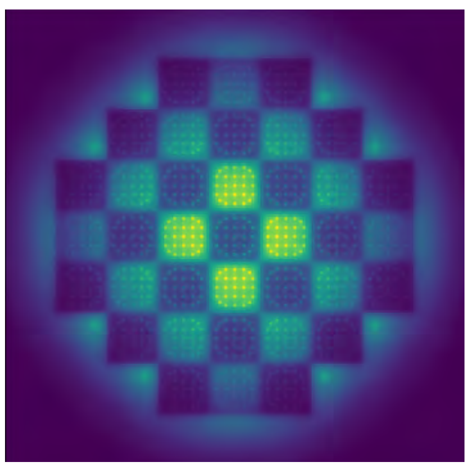


Figure 2. Thermal flux in the SMR problem calculated in MC/DC.

There are a variety of approaches and methods that can be used for solving particle transport problems in different physical applications. Each particle transport problem has its specific features that should be considered in developing accurate and efficient computational methods. Major challenges of particle transport problems that keep us striving for ever-improving computational methods include: the high dimensionality of the phase space; multiple scales in time, space, and energy; strong nonlinearities; the natural endeavor to obtain continuously greater resolution; the addition of more and more physics; and the ever-changing architecture of computers. Novel high-performance computing systems bring bright new opportunities as well as challenges.

The Center for Exascale Monte Carlo Neutron Transport (CEMeNT) focuses on developing innovative numerical methods and computer algorithms for time-dependent neutron transport problems, with an eye toward benefitting the solution of general problems of various kind of particles, on exascale computing architectures and for a spectrum of physical applications relevant to the Department of Energy/National Nuclear Security Administration (DOE/NNSA) mission. The CEMeNT team consists of researchers from Oregon State University, North Carolina State University, and the University of Notre Dame and brings together experts in computational physics and engineering, applied mathematics, nuclear simulations, computer science, and high-performance computing. The solid concrete block of CEMeNT is the group of eight graduate students from the three university partners and two postdoctoral researchers. The team has created an open-source Python-based Monte Carlo (MC) code, MC/DC, for time-dependent transport problems. This software is used to implement, analyze, and test computational methods and algorithms under development. CEMeNT researchers have modified the advanced MC transport code, Shift, created by Oak Ridge National Laboratory, amplifying its existing, formidable capabilities to solve time-dependent problems. The team uses the library of finite element methods in the MFEM package from Lawrence Livermore National Laboratory as a high-performance software toolbox to explore hybrid MC/deterministic numerical algorithms.

The Center has made significant progress in several directions of its research. The team implemented time-dependent simulation modes in the central processing unit (CPU)- and graphics processing unit (GPU)-codebases of Shift with execution verified on the AZURV1 benchmark and validated using the first Shift simulations of the pulsed sphere experiments. A novel, on-GPU, asynchronously scheduled runtime framework was developed and found to efficiently reduce divergence by remapping in shared memory and processing events opportunistically. Performance of CEMeNT's Python Monte Carlo transport code, MC/DC (Figure 1), has been improved by implementing the Numba just-in-time compilation technique, while keeping the scalability of MPI4Py. Abstraction for integration of Numba-based OpenMP threading and GPU techniques also is underway. The Center has identified a challenge problem—a generic small modular reactor (SMR—to formulate baseline performance metrics in both code bases (Shift and MC/DC) for steady-state, eigenvalue, and time-dependent modes (Figure 2). Novel Quasi Monte Carlo (QMC) methods for transport problems have been developed, and the team works on implementing QMC techniques into MC/DC utilizing the MFEM deterministic solver. All CEMeNT graduate students have had an internship at one of NNSA labs, working with leading experts in the field and their research groups.

Integrated Simulations Using Exascale Multiphysics Ensembles | Stanford University

PI: Dr. Gianluca Iaccarino (jops@stanford.edu); Authors: Kazuki Maeda and Thiago Teixeira

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 complex, multi-physics phenomena by combining innovative, task-based programming, implicit parallelism, physical modeling, numerical algorithms, data analysis, learning-at-scale, and uncertainty quantification. The Center is comprised of faculty and researchers from Stanford, the University of Colorado Boulder, and Purdue University.

The overarching goal of the Center is predicting the reliability of the laser-based ignition (LBI) of a methane-fueled rocket engine operated at high altitudes. Successful and repeatable ignition is key to attitude control and injection of spacecrafts in orbit. LBI employs miniaturized, nano-second, high-energy laser pulses and is a promising technology under active development in the aerospace industry. Critical reliability assessments of LBI rely mostly on physical prototyping. The Center's goal is to enable simulation-based predictions of ignition reliability by means of multi-physics simulations using a novel software framework that is portable across exascale machines with heterogeneous architectures.

The Center's strategy for the reliability prediction is based on multi-fidelity ensemble—simultaneous execution of many simulations at various levels of physical fidelity. Implicit parallelism using the Legion programming model is at the core of this strategy. Using Regent, a high-level language for task-based programming in Legion, we aim to achieve parallel performance of the complex simulations on heterogeneous systems with minimal tuning. This software design enables rapid integration of model development, implementation, simulation at scale, and data analysis on state-of-the-art central processing unit/graphics processing unit (CPU/GPU) leadership-class supercomputers.

The technical objective is to produce ignition probability maps in the combustor from an ensemble of up to O(1M) simulation members. The simulation methods are designed at various levels of fidelity and cost, ranging from three-dimensional Large Eddy Simulations (LES) to reduced, machine-learned surrogate models. The simulations are carefully verified and validated by companion experiments. The ignition probability accounts for intrinsic uncertainties in the system, including variabilities in laser energy/position, deposition time/interval, propellant inflow conditions, chamber condition/geometry, etc. To this end, in the second year of the Center's operation, efforts made in the first year have been continued/extended on 1) full-system simulations on GPUs using an in-house, compressible reacting flow solver, 2) verification of the solver accuracy, 3) design of a Legion-based automapper to accelerate ensemble simulations, 4) deployment of continuous integration/continuous delivery (CI/CD) methodology to enhance software portability, 5) design of Legion-based ensemble coprocessing, 6) multiblock grid capabilities in the solver, 7) development of an interactive browsing tool for the analysis of ensemble data, 8) development of data-driven models for spray atomization, 9) construction of the probability map by experiments, and 10) experimental validation of simulations. In addition, to further explore strategies for software integration and Legion-based ensembles, a new task-based framework has been designed for multi-fidelity ensemble simulations and in situ data processing. The framework features a Regent solver for simulations and a Pygion-API for data processing using general-purpose Python libraries. A mini-app built on this framework has been ported to different architectures, including Tioga at Lawrence Livermore National Laboratory, the latest AMD CPU/GPU system.

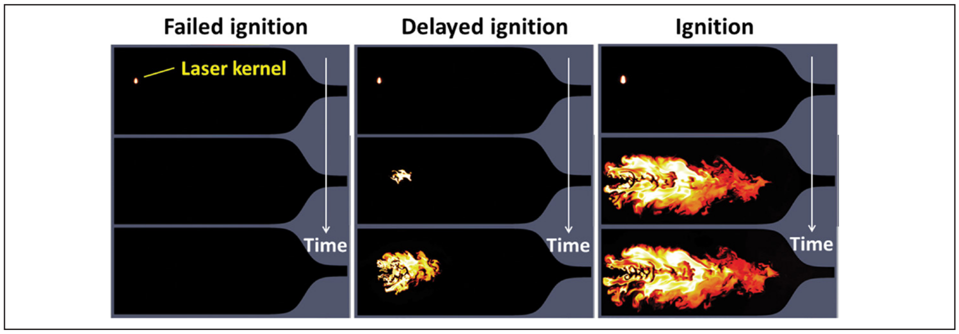


Figure 1. Evolution of the cross-sectional temperature fields of the INSIEME PSAAPIII rocket combustor prototype simulated on GPUs of LLNL's Lassen Supercomputer for cases indicating (left) failed ignition, (center) delayed ignition, and (right) standard ignition. Ignition failure/delay depends on the laser-amplitude and stochasticity.

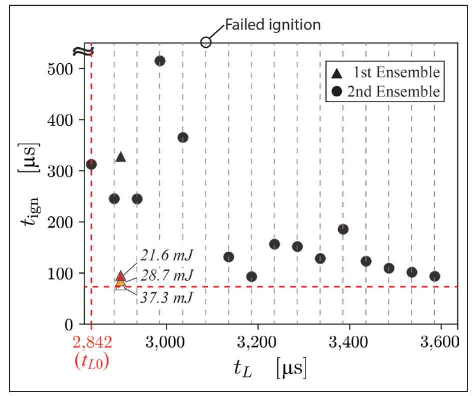


Figure 2. Scatter plot of the ignition delay time (t_{ign}) against the laser deployment time (t_L), obtained from ensemble simulations of the combustor shown in Figure 1. The negative correlation of t_{ign} and t_L, can be explained by the slower quenching/dissipation of the ignition kernel in the propellant jet at greater t_L, due to combustor pressurization and resulting deceleration of the jet.

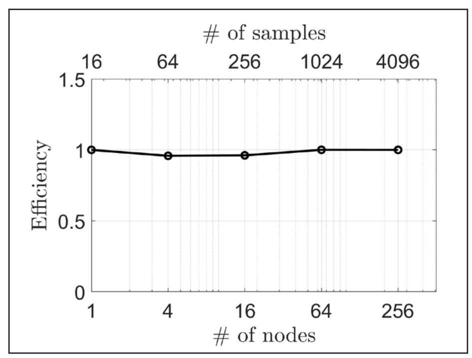


Figure 3. Mini-app's weak scaling of ensemble simulations on GPUs of Lassen. Four samples are mapped on each GPU with 3.2 M grid cells per sample. Excellent scaling is obtained for up to 256 nodes (1024 GPUs, 13.1 B total grid cells).

We look forward to the third year of the PSAAP III program and are excited about further research advancements.

The Center for Hybrid Rocket Exascale Simulation Technology | University of Buffalo

PI: Dr. Paul Desjardin (ped3@buffalo.edu)

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.

The primary effort of the Center over the first two years has been experimental and numerical analysis of a well characterized small scale slab burner. The insights from the slab burner experimental work, along with uncertainty analysis of measurements, has driven the development of CHREST's collaborative software framework, Ablative Boundary Layers At The Exascale (ABLATE). The opensource exascale framework ABLATE (ablate.dev) consists of low- and high-Mach CFD solvers, radiation solver, prediction assessment modules, flows, and several subgrid scale models to account for shear-driven atomization and turbulent combustion phenomena.

As the Center moves past these preliminary efforts, focus is shifting to applying the insights and software developed to real world applications including modeling the National Aeronautics and Space Administration (NASA) Ames Peregrine hybrid rocket motor. Figure 1 of the NASA Ames Peregrine motor modeling using ABLATE shows the turbulent reacting environment inside of the hybrid rocket. As part of CHREST undergraduate research efforts, tools have been developed in ABLATE for collecting propulsion and turbulent run-time statistics. Resolving the required physics for these models requires high performance computing resources such as the UB Center for Computational Research (UBCCR) and LLNL Quartz,

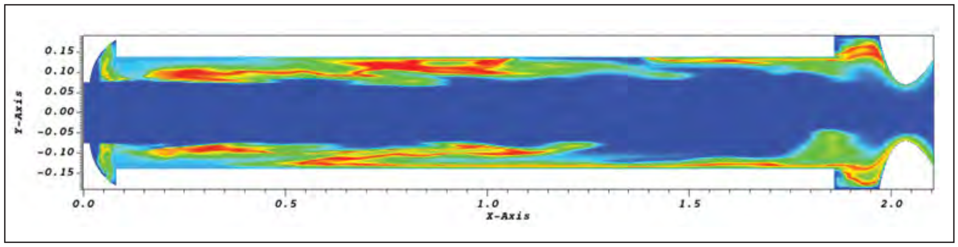


Figure 1. Preliminary simulations of the Peregrine Hybrid Rocket Motor using the ABLATE framework performed by CHREST undergraduate student Salam Lobad.

the later of which was utilized for the simulations shown in Figure 1. 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.

Education has been a primary focus at CHREST with an emphasis in areas ranging from undergraduate education to National Nuclear Security Administration (NNSA) laboratory internships. Highlights include the newly developed, open-source, new researcher ABLATE boot camp (coding. ablate.dev). This day-by-day guide is tailored to help onboard individuals with little to no programming experience using a 20-day online course. This course is designed to take a few hours every day and includes selected book chapters, online tutorials, videos, and manual excerpts.

CHREST graduate researchers, Mae Sementilli and Venus Amiri (Figure 2), have completed NNSA laboratory internships at Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory (LLNL), respectively. At her internship this past summer at LANL, Mae had the opportunity to work on the solver methodology for the multiphase flow capabilities of ABLATE. The advisors with whom she worked have specialized knowledge in this area of computational fluid dynamics, resulting in key insights into the equations of state utilized. This internship helped overcome an obstacle in development, which is now leading to accelerated progress in shear-driven flow research. Venus began her internship at LLNL in the area of chemical kinetic modeling. She

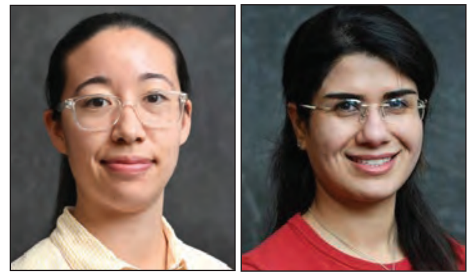


Figure 2. Mae Sementilli and Venus Amiri completed NNSA laboratory internships at Los Alamos National Laboratory and Lawrence Livermore National Laboratory, respectively.

is working on an automatic generation mechanism, and this opportunity improved her understanding of both thermochemistry and chemical kinetics by learning from the experts in the field. Since LLNL is one of the pioneers in this area, this internship broadened her critical view for mechanism generation of paraffin which will be employed for the slab burner modeling. Their knowledge and insights gained at the NNSA internships have proven invaluable to the continued research efforts at CHREST.

More details can be found at: https:// buffalo.edu/chrest.

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)

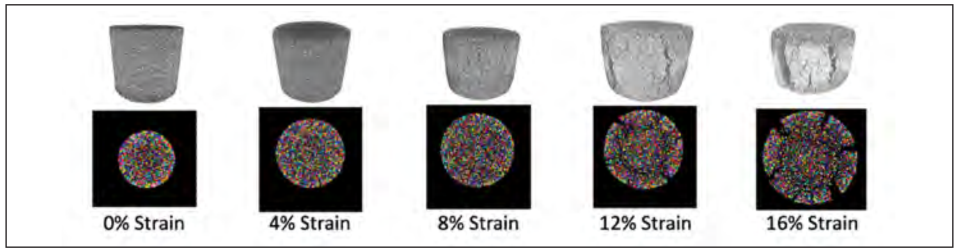


Figure 1. Application of Segmentflow (Becker, Mines) to track deformation from CT images of unconfined compression experiments on mock HE (Lu, UT Dallas).

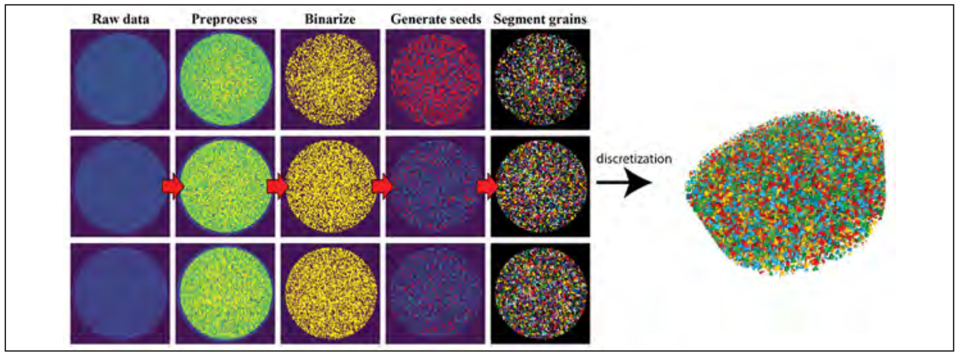


Figure 2. Development and application of Segmentflow python code to process CT data into images used for initial spatial discretization of Finite Element (FE), Discrete Element (DE), and Material Point Method (MPM) simulations (Becker, Mines).

The long-term 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 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 high-speed imaging. The mock HE is composed of a mixture of approximately 1 millimeter diameter agglomerated prills of idoxuridine (IDOX) (average grain diameter approximately 200 micrometers) mixed with polymeric Estane binder. A secondary mock is composed of F-50 silica sand (average grain diameter approximately 350 micrometers) mixed with polymeric FK-800 resin. The Year 5 objective is to predict with quantified uncertainty the compressive mechanical behavior of pressed, recycled mock HE at medium strain rate (using a gleeble thermo-mechanical device) within a computational multiscale, calibrated-and-validated-Direct-Numerical-Simulation-(DNS)-informed, micromorphic continuum mechanics framework. The main question the MSC is attempting to answer is whether it can predict at higher fidelity—compared to classical continuum mechanics---the compressive mechanical behavior of pressed, recycled mock HE at various strain rates within a computational multiscale, micromorphic continuum mechanics framework.

Some highlights from Year 2 include: (i) establishing Integration and Workflows across the press manufacturing mechanical experiments (single grain compression at quasi-static and high strain rates, 0.2 inch and 0.5 inch diameter cylindrical specimens compressed at quasi-static, intermediate, and high strain rates), CT imaging at various stages of loading (see Figure 1), multiscale modeling, machine learning, computational simulation, Uncertainty Quantification (UQ), and exascale computer science research activities; (ii) forming Integrated Task Teams (ITTs) to push forward these research activities into smaller coordinated efforts to meet the annual predictive simulation; (iii) Segmentflow (see Figure 2, https://gitlab.com/micromorph/segmentflow) written to process CT data and convert to input numerical spatial discretizations for Finite Element (FE), Discrete Element (DE), and Material Point Method (MPM) simulations; (iv) simulation of press manufacturing using LAMMPS-granular (see Figure 3); (v) Ratel GPU FE code demonstrates performance on Crusher, Summit, Lassen, and Perlmutter; and (vi) demonstration of Tardigrade micromorphic-upscaling in preparation for annual predictive simulation.

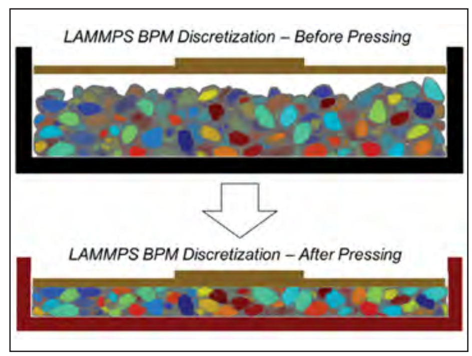


Figure 3. LAMMPS simulation of pressing manufacturing of mock HE (Lamont, CU Boulder).

Certain MSC activities for FY 2023 include: (1) annual predictive simulation of 5mm diameter pressed cylinders mock HE; (2) development of implicit MPM for quasi-static large deformation, fracture, and fragmentation simulations; (3) micromorphic upscaling within Tardigrade for annual predictive simulation; (4) continued experiments with in-situ CT or pre- and post-CT imaging along with segmentation via Segmentflow to generate grain statistics to validate computational simulations against experimental results.

For more information, visit micromorph.gitlab.io).

The Center for Exascale-enabled Scramjet Design | University of Illinois at Urbana-Champaign

PI: Dr. Jonathan Freund, jbfreund@illinois.edu; Co-director: Dr. William Gropp, wgropp@illinois.edu

This Predictive Science Academic Alliance Program (PSAAP) Center is using predictive science to advance scramjet technology through designs that incorporate novel, lightweight, fiber composite, combustor materials. In its second year, the Center currently supports 16 PhD students, and has so far placed one former student in a position at a National Nuclear Security Administration (NNSA) laboratory. To date, six current PhD students plus two recent students have completed 10-week internships at NNSA laboratories, several of which have led to ongoing collaborations with laboratory personnel. The number of internships and placements is expected to grow, since a high number of students started their graduate studies at the start of the grant. Professor Freund remarks that "PSAAP Centers are unique in how they train students within a broad predictive science environment, allowing the evaluation of high-risk research concepts within a larger context."

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 evaluation of novel composite materials. How these materials interact with the flow in the supersonic core of the combustor is central to the design process. To assess this predictively, physical models are being integrated for gas-phase turbulent combustion, 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 being developed synergistically with physics-targeted experiments for calibration and validation (Figure 1). The Center's end-to-end uncertainty quantification workflow leverages the low-dimensional, physics-targeted configurations for reduction of the uncertainty space through sensitivity analysis. Experimental data from the ACT-II supersonic combustion facility on the Illinois campus is providing the Center's integrated-physics annual prediction targets.

For resolving the multiple time and length scales of the physics, a novel computational framework has been constructed around tools designed in the Center along with community tools. The governing equations are expressed in Python, exposing computational kernels of the discretization. These kernels are flexible in their expression and adhere to straightforward rules. They are human readable, crafted by the computational scientists and those implementing the details of the numerical discretization. To enable portable performance at scale, the computational kernels then are processed automatically into a polyhedral loop abstraction, which allows them to be 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.

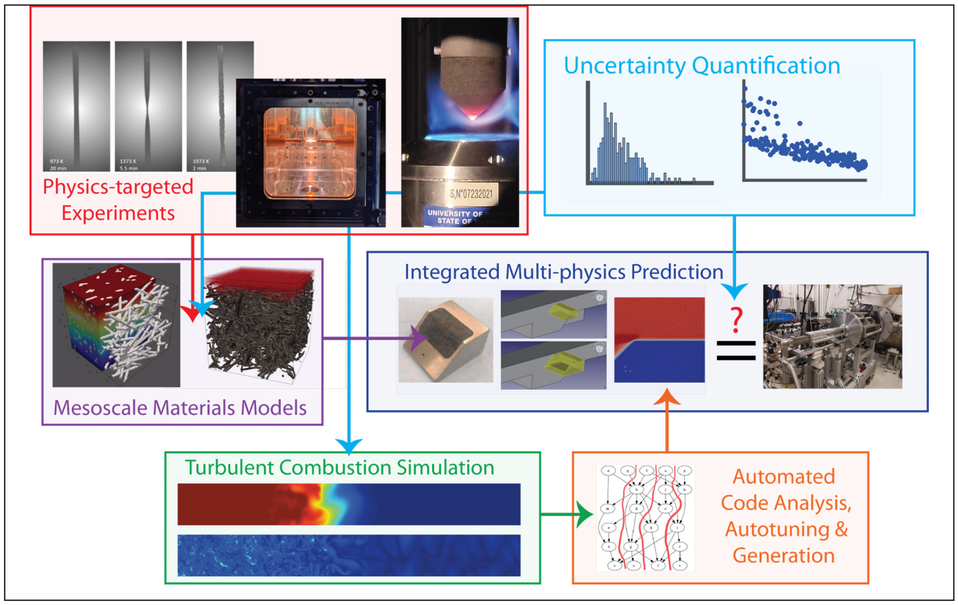


Figure 1. High-level schematic of the physics-targeted experiments, mesoscale materials models, turbulent combustion simulations, and computer science tools that integrate the Center's effort into its predictions within the uncertainty quantification framework.

In this framework, the Center has developed MIRGE-Com, a new Discontinuous Galerkin flow and combustion solver, and an initial lazy evaluation traversal of it has been demonstrated to generate code, avoiding the need to manually develop code for specific machines. For example, MIRGE-Com executes on local machines, LLNL Quartz CPUs, and Lassen GPUs. Another Illinois tool, Pyrometheus, generates lightweight code for specific combustion chemistry based on the extensive Cantera combustion kinetics package. The lazy evaluation procedures accelerate the combustion routines by a factor of nearly 100 relative to a baseline implementation. For making predictions, meshing, and simulation workflow has been established, and the workflow management tool Parsl is being extended and evaluated for orchestrating multi-stage simulation and uncertainty quantification workflows with the option of interacting with simulation runs through Jupyter notebooks. New non-expert users have successfully implemented methods for shock capturing, limiting, and additional governing equations (e.g., the heat equation), demonstrating the accessibility of the computational-science-facing Python drivers of the framework. Daily verification tests cover nearly all code during development, and the historical performance is tracked for simulations representative of anticipated annual predictions.

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 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, as illustrated in Figure 1. Existing methods for sensitivity computation generally fail for chaotic problems due to the “butterfly effect” which amplifies infinitesimal disturbances beyond bound.

One of the focal points of the research is to extend the so-called “space-split sensitivity” (S3) method to turbulence problems. This method is theoretically grounded in linear response theory but, before now, had only been applied to problems like chaotic maps. During the last year, Adam Sliwiak (PhD student) extended the S3 method to systems of ordinary differential equations (the Lorenz equations) and partial differential equations (the Kuramoto-Sivashinsky equation, shown in Figure 2). He now is working with Nikhil Oberoi (PhD student) to apply the S3 method to a turbulent channel flow. This will be a very important step and an important test of the method, as this constitutes a “real” turbulent flow (albeit a highly canonical one).

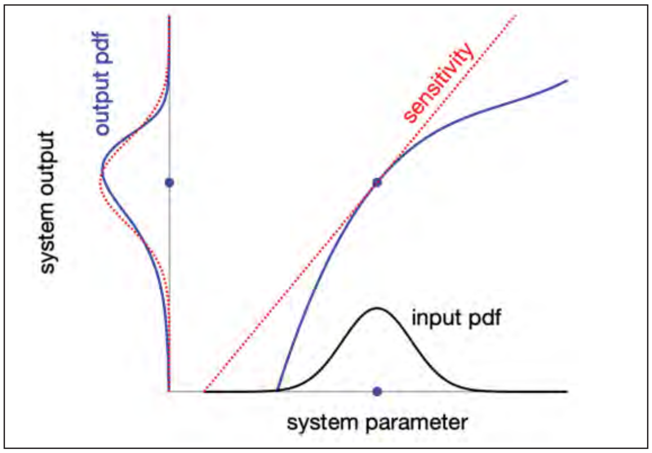


Figure 1. The sensitivity of a system is the gradient in parameter space. It allows for approximate estimation of how input uncertainties propagate to the output.

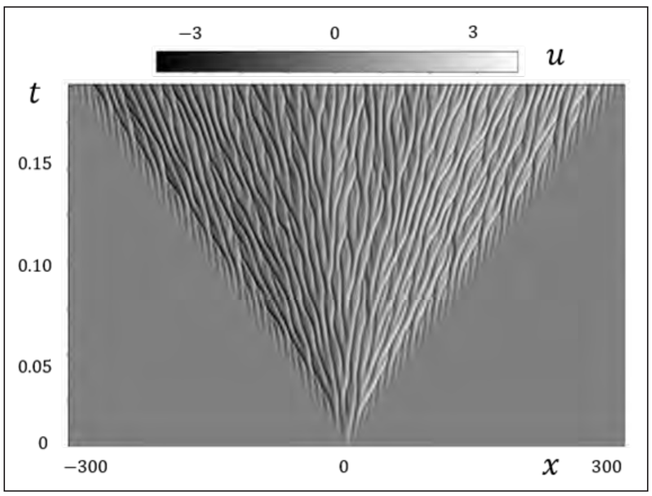


Figure 2. A solution to the Kuramoto-Sivashinsky partial differential equation which produces chaotic solutions in a low-dimensional context.

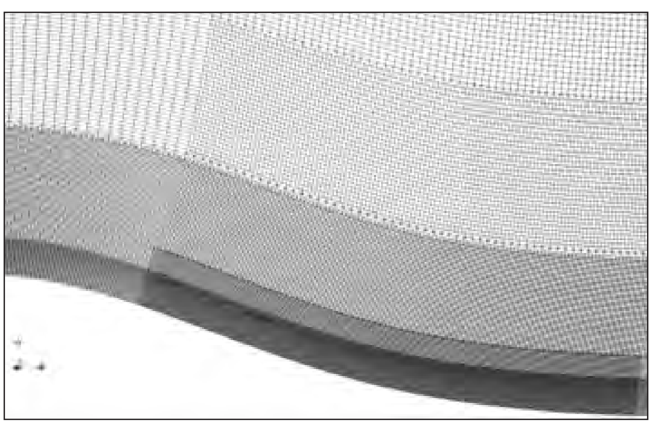


Figure 3. A computational grid for the flow over a smooth bump, adapted from an initial ignorant grid according to the error estimator and grid-adaptation methodology.

The Center also is pursuing a second approach to sensitivity estimation that is based on ideas from turbulence modeling. Specifically, in this approach, the Center defines an approximate time-averaged problem from the high-fidelity turbulence data and, then, explore the sensitivity of that approximate problem. The approximation requires modeling assumption that will affect the accuracy of the sensitivity. During the last year, Walter Arias Ramirez and Nikhil Oberoi (both PhD students) finalized assessment and validation of the first attempt at sensitivity estimation within this paradigm on the flow over an airfoil and a supersonic shock/ boundary-layer interaction.

In parallel, the Center is highly focused on the problem of error estimation in turbulence simulations, specifically on estimating how the computational grid creates errors in the solution. During the last year, Ali Kahraman (PhD student) has shown how to implement the most promising error estimator in a high-order, finite-element-type code and how this leads to a successful grid-adaptation methodology. The demonstration cases include different channel flows and the flow over an airfoil. Going forward, the Center will explore ways to use the error estimation techniques to produce better computational grids for turbulence simulations and for different types of grid topologies (Figure 3).

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

PI: Dr. Patrick Bridges (patrickb@unm.edu)

The Predictive Science Academic Alliance Program III (PSAAP-III) Center and the University of New Mexico (UNM), University of Tennessee at Chattanooga (UTC), and the University of Alabama (UA) focus on improving the communication systems that underpin all modern supercomputing systems. To do so, it focuses on characterizing the communication behaviors of state-of-the-art, Department of Energy (DOE) applications and systems, creating and optimizing new communication abstractions for these systems, and modeling and making transparent the performance of these primitives so that applications and runtimes can use them effectively. Seven graduate students and one postdoctoral fellow are funded across the academic institutions comprising this Center, and four project alumni have joined National Nuclear Security Administration (NNSA) laboratories as staff or postdoctoral fellows.

A key focus this year has been on graphics processing unit (GPU) communication. First, Center researchers examined and optimized performance of the Los Alamos National Laboratory HIGRAD and UNM FIESTA research codes to provide an upper bound on optimized regular halo communication performance. Personnel optimized HIGRAD to minimize data packing overheads and send data directly from the GPU and modified both HIGRAD and FIESTA to use either hand-packed communication buffers or library datatype handling. Results demonstrated that current library datatype primitives decreased performance by more than a factor of four, while application data-packing approaches and CUDA-aware communication improved HIGRAD performance by more than 25%. These results provide important guidance for new library communication primitives.

Center personnel also examined GPU-triggered communication to minimize GPU/network interface controller (NIC) synchronization and handoff latencies. Results demonstrated that the upfront cost of setting up the triggered communication needs to be overlapped with computational kernels (Figure 1) and that unexpected messages can cause a 10x performance hit. As shown in Figure 2, a three-dimensional stencil halo exchange that sends 26 messages triggered communication resulted in a 2% performance gain, whereas an exchange with six messages and implicitly sends edges and corners resulted in a 11% performance gain. Together, these highlight the need for new communication primitives and implementations that can provide these benefits to applications.

Center personnel have been working on the partitioned, point-to-point communication primitives introduced in the message passing interface (MPI) 4.0 standard to support hybrid communication approaches. These enable MPI libraries to transfer parts of data buffers as application threads or GPU warps complete. Center personnel designed, implemented, and evaluated a layered library implementation of these newer application programming interfaces (APIs) that use either persistent point-to-point primitives or remote-memory-access (RMA) primitives and evaluated their performance against traditional single- and multi-send methods for large buffer sizes. The results[1] demonstrated a trade-off where the RMA implementation was better for send-side partitioning, and persistent-based communication was better for receive-side partitioning. Specifically, RMA send-side partitioning increased perceived bandwidth 8.9x over a single send compared to 4.0x for persistent-based send-side partitioning, whereas persistent-based receive-side partitioning provided up to 5.37x higher overlap than RMA.

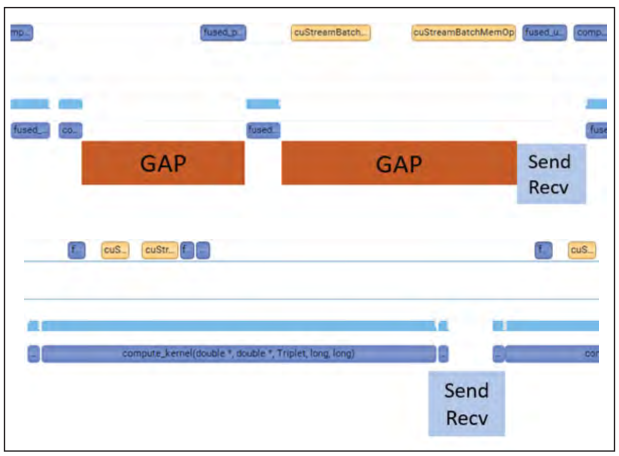


Figure 1. NVIDIA NSYS traces comparing of a GPU-triggered sends with short (top) and a long (bottom) compute kernel

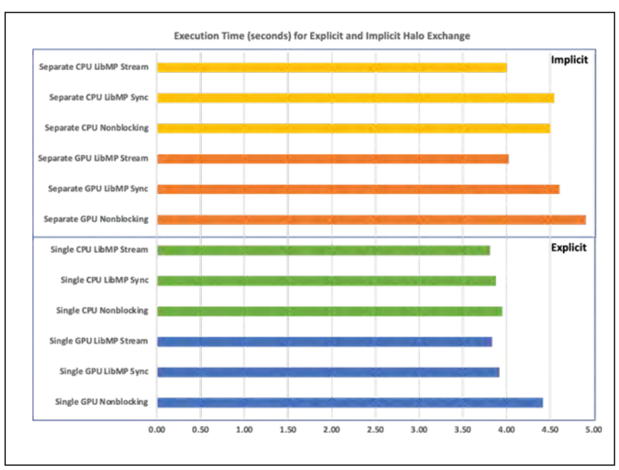


Figure 2. Performance of various GPU-triggered halo exchange approaches

Finally, the Center has made new communication abstractions and optimizations, such as partitioned and locality-aware communication, publicly available through the MPI Advance framework.[2] MPI Advance provides open source optimizations to partitioned communication neighborhood collectives and basic collective operations. These codebases utilize the MPI profiling library so that optimizations can be easily added into existing applications with minimal changes, regardless of the available system MPI.

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[2]Anthony Skjellum, Purushotham V. Bangalore, Derek Schafer, and Amanda Bienz. MPI-Advance. https://github.com/mpi-advance

Exascale Predictive Simulation of Inductively Coupled Plasma Torches | The University of Texas at Austin

PI: Dr. Robert Moser (rmoser@oden.utexas.edu)

The Center for Predictive Engineering and Computational Sciences (PECOS) in the Oden Institute for Computational Engineering and Sciences at The University of Texas (UT) is the home of a Predictive Science Academic Alliance III (PSAAP III) Center focused on the simulation of an inductively coupled plasma (ICP) torch. The PSAAP project, which is just finishing its second year, is an integrated computational and experimental campaign to develop predictive computational models of a plasma torch device that is installed in the Flow Field Imaging Laboratory at UT and is shown in operation in Figure 1. Such devices can operate with a variety of feed gases and are used in laboratory and industrial applications in which a clean plasma is needed. The device at UT is used for ablative material testing for reentry vehicles. As a modeling target, the ICP torch also is a surrogate for highly-collisional plasmas in a variety of other applications. The Center currently is supporting 14 graduate students and five postdoctoral scholars who are working with 14 faculty and senior researchers from five different departments at UT.

Predictive simulation capability for an ICP torch requires numerous developments in modeling, validation and uncertainty quantification, computational mathematics, and computer science. To enable simulations of the torch operating on argon, this year an initial three-dimensional, time-dependent argon plasma model was implemented in the mixed finite element method (MFEM) finite element infrastructure from Lawrence Livermore National Laboratory (https://mfem.org/). The plasma is modeled as a quasi-neutral, multi-component (including electrons), reacting gas in which the electrons are not in thermal equilibrium with the heavy species, requiring a separate energy equation for electrons. Because electrons are not in thermal equilibrium, electron impact reaction rates and electron transport properties are determined from solutions of the spatially homogeneous Boltzmann equation given representations of collision cross-sections. The transport equations are discretized with a

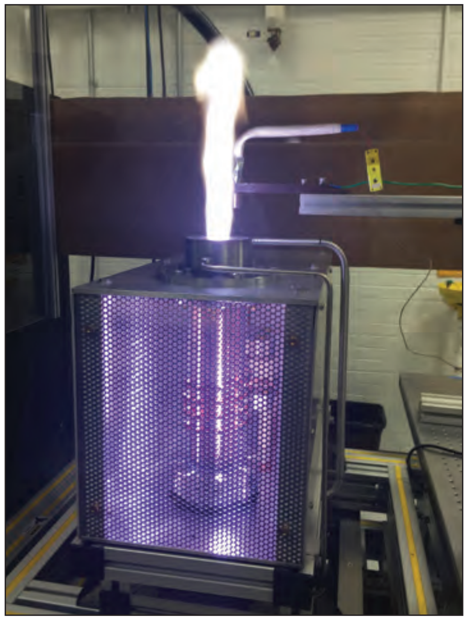

Figure 1. The 50 kW inductively-coupled plasma torch in the Flowfield Imaging Lab at The University of Texas here shown operating with air as the feed gas.

high-order discontinuous Galerkin formulation and implemented using MFEM macros for execution on both central and graphics processing units.

Many of the model inputs to the torch simulation (e.g., collision cross-sections, transport coefficients, boundary conditions) have significant uncertainties, and reliable predictions require that these uncertainties and their impact be characterized. Of particular importance are the electron-impact collision cross-sections which are functions of the collision energy. Data for these cross-sections are available from electron-beam experiments and *ab-initio* quantum calculations, but there are large discrepancies among these data that cannot be explained by their reported uncertainties. These cross-sections are represented as a function of energy using semi-empirical models with uncertain parameters. To represent the uncertainties implied by the unexplained discrepancies in the data, the semi-empirical models are augmented with Gaussian process models, and the model parameters and hyperparameters are determined by Bayesian inference. As shown in the example in Figure 2, the uncertain cross-section model provides a good characterization of the data

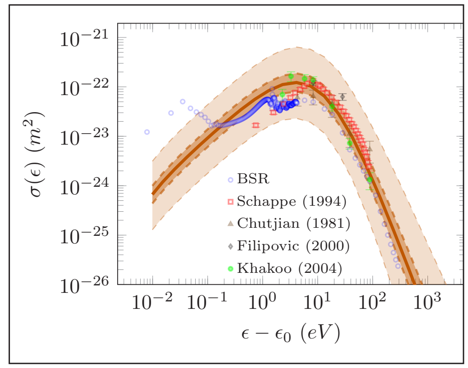

Figure 2. Argon-electron collision cross sections for the 1s3 transition as a function of energy where ε_0 is the excitation threshold (11.72 eV). Shown are the mean (solid line) and the 68% and 99% confidence intervals of the Gaussian-process, semi-empirical model. Also shown are data from ab initio calculations (BSR) and four different electron-beam experiments.

discrepancies. The model has also been validated against swarm experiments.

Propagating these input uncertainties to ICP torch model predictions is challenging, because the torch simulator is computationally expensive. Multi-fidelity Monte Carlo uncertainty quantification algorithms, which allow most of the sampling to be done using less expensive, lower order models, are being used to address this challenge. In particular, best linear unbiased estimators are used which are provably optimal. These algorithms have been enhanced by reformulating the optimization problem required to setup the multi-fidelity sampling, so that it can be solved efficiently and account for multiple output quantities of interest.

The developments described are being used to perform simulations of the ICP torch to predict the outlet plasma conditions. The accuracy of the predictions will be assessed by comparison to temperature and composition measurements in the Flow Field Imaging Laboratory.

Hillary Fairbanks, Lawrence Livermore National Laboratory (fairbanks5@llnl.gov) ✦ **Years at LLNL:** 2018-Present
Degree: PhD, Applied Mathematics ✦ **PSAAP:** 2013-2017, University of Colorado Boulder

I was involved in the Predictive Science Academic Alliance Program (PSAAP) II project at the University of Colorado Boulder from 2013-2017. The goal was to develop numerical methods to model particle-based solar receivers with an aim to better understand the underlying physical processes and to improve energy efficiency. I joined in my second year of graduate school when my research group (led by Prof. Alireza Doostan, my PhD advisor) was tasked with developing efficient, multi-fidelity algorithms to perform uncertainty quantification (UQ) on the corresponding large-scale, turbulent flow models. In our work, we investigated how exploiting low-fidelity solvers could help speed up UQ performance for our application with minimal loss of accuracy. This work resulted in three publications,[1,2,3] the final of which focused on characterizing uncertainties for the irradiated, particle-laden turbulent flow problem.

In addition to working on an interesting and challenging problem, the PSAAP II project provided me with an opportunity to engage with the broader academic and national laboratory communities. I had the opportunity to attend several conferences to present our work and to attend workshops to strengthen my own research skills. As part of the program, I interned at one of the National Nuclear Security Administration (NNSA) labs, Lawrence Livermore National Laboratory (LLNL), with Dr. Panayot Vassilevski. For this research, we worked on developing approaches to accelerate multilevel Monte Carlo and later scalable multilevel approaches for Bayesian inference (this work was submitted after my graduation).[4] This opportunity provided additional exposure to the high-performance computing environments at the core of large-scale scientific computing.

It was because of this internship and my interest in learning more about scalable computing for uncertainty quantification, that I joined LLNL as a postdoctoral fellow (postdoc) following graduation. Upon completing my postdoc, I joined as a staff member at the Center for Applied Scientific Computing. I continue to work in the development of algorithms and software for large-scale, predictive simulations with a focus on scalable multilevel and multigrid approaches to accelerate UQ. The work I did with the PSAAP II project was foundational to the applications and problems I work on at LLNL, and I am very grateful for the opportunities that it has provided for me.

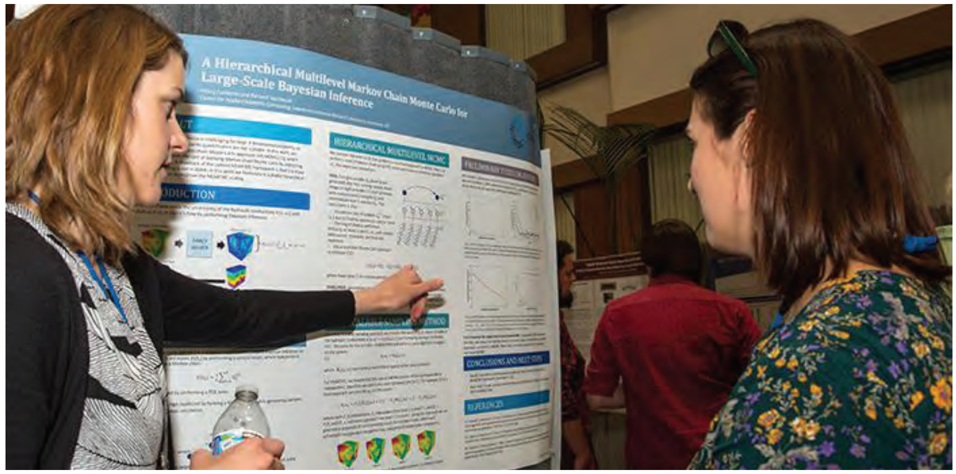

Figure 1. Fairbanks presents a poster at the 12th Annual Postdoc Poster Symposium at Lawrence Livermore National Laboratory (LLNL). The poster, entitled "A Hierarchical Multilevel Markov Chain Monte Carlo for Large-Scale Bayesian Inference" describes research she completed during her postdoc.[5] Photo courtesy of LLNL

In addition to working on an interesting and challenging problem, the PSAAP II project provided me with an opportunity to engage with the broader academic and national laboratory communities. I had the opportunity to attend several conferences to present our work and to attend workshops to strengthen my own research skills. As part of the program, I interned at one of the National Nuclear Security Administration (NNSA) labs, Lawrence Livermore National Laboratory (LLNL), with Dr. Panayot Vassilevski. ... It was because of this internship and my interest in learning more about scalable computing for uncertainty quantification, that I joined LLNL as a postdoctoral fellow (postdoc) following graduation. Upon completing my postdoc, I joined as a staff member at the Center for Applied Scientific Computing.

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[5]H.R. Fairbanks, U. Villa, and P.S. Vassilevski. "Multilevel Hierarchical Decomposition of Finite Element White Noise with Application to Multilevel Markov Chain Monte Carlo," SIAM Journal on Scientific Computing 43(5), S293-316 (2021).

Robert Knaus (rcknaus@sandia.gov), Sandia National Laboratories ✦ **Years at SNL:** 2015-Present
Degree: PhD, Mechanical Engineering; Computational Math, Science, and Engineering
PSAAP: 2014-2015, University of Illinois at Urbana-Champaign

My research at the Predictive Science Academic Alliance Program (PSAAP) Center for Exascale Simulation of Plasma-coupled Combustion (XPACC) focused on simulating a feature of turbulent combustion where, at sufficiently high speeds, regions of local quenching occur increasing the pollutants produced by the combustion process and reducing its efficiency. As part of XPACC, I worked at Sandia National Laboratories (Sandia) as a graduate student intern in the PSAAP internship program. During the internship, I integrated my thesis work into an open-source software developed at Sandia. This allowed the capability I developed to be generalized to the complex geometries of real combustion systems. It also gave me the opportunity to work with and receive mentorship from leading experts in computational modeling for predicting fires. The time at Sandia convinced me that I would enjoy working at a Department of Energy/National Nuclear Security Administration (DOE/NNSA) laboratory in a collaborative team environment with access to broad computational resources and support and the ability to make an impact on solving important national security problems. I learned modern software development practices and other skills that helped me in the remainder of my graduate studies at the University of Illinois and my career after. The internship allowed me to network across the lab and to find a place that aligned with my interests. After completing my graduate studies, I joined Sandia as a postdoctoral researcher before converting to staff.

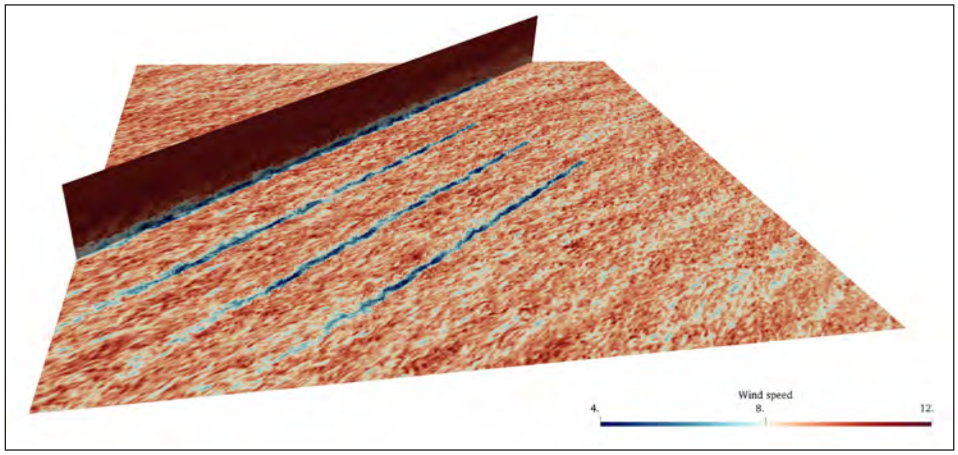


Figure 1. Simulation of a wind farm in an atmospheric boundary layer with wind turbines modeled through an "actuator line" model. "Actuator lines" describe the effect of a turbine on the wind through a modeled force term, allowing for more computationally tractable predictions.

As a staff member at Sandia, I develop software for predicting the dynamics of large-scale thermal and fluid systems; for instance, simulating a fire resulting from a fuel spill or simulating the wind past an array of wind turbines. These systems involve solving equations relating to atmospheric dynamics, thermal radiation, conjugate heat transfer, chemical reactions, fluid/structure interactions, wave modeling, variable density turbulence, and more. As a developer at Sandia, I work on a software development team with many talented developers to deliver high-quality, verified, and validated software to provide a trustworthy computational capability that can take full advantage of the latest supercomputing hardware. I interface with users and support them tackling difficult and cutting-edge research problems. I also pursue research into new physics models and numerical algorithms to push the limits on what we achieve with our software stack.

Working at Sandia allows me to work with many talented people to help solve national security problems. The broad set of work means that I can work on cutting edge research problems that interest me.

As part of XPACC, I worked at Sandia National Laboratories (Sandia) as a graduate student intern in the PSAAP internship program. ... The time at Sandia convinced me that I would enjoy working at a Department of Energy/National Nuclear Security Administration (DOE/NNSA) laboratory in a collaborative team environment with access to broad computational resources and support and the ability to make an impact on solving important national security problems. I learned modern software development practices and other skills that helped me in the remainder of my graduate studies at the University of Illinois and my career after.

Gerald Collom (geraldc@unm.edu)
Degree in Progress: PhD, Computer Science, University of New Mexico ✦ Advisor: Dr. Amanda Bienz ✦ PSAAP: 2020-Present

Research Topic

High Performance Computing Communication

Research Responsibilities

I perform research under the supervision of Prof. Bienz on optimizing communication for high performance scientific computing applications. This includes assessing Department of Energy (DOE) application needs, examining new communication primitives for DOE algorithms, and assisting with the research and development of new models and implementations of these primitives.

Benefits of PSAAP

The Predictive Science Academic Alliance Program (PSAAP) is responsible for making my graduate studies a possibility. Simply put, without PSAAP, I would not have had the opportunity to pursue a PhD and a career in research, as I am entirely self-funded without any help from family or elsewhere. Beyond making my pursuits possible, participation in PSAAP has given me numerous opportunities. I have had the opportunity to intern at Lawrence Livermore National Laboratory (LLNL) for two summers, and each was incredibly educating and experience building. Furthermore, attending a PSAAP meetup exposed me to a wide variety of fascinating research and opened the chance for connections that I wouldn't have otherwise made. This has led to new research directions and professional acquaintances.

National Laboratory Experience

I spent two summers interning at LLNL and have collaborated with national laboratory scientists throughout my graduate program. These opportunities have presented new research topics to me and enriched my background knowledge in high performance computing (HPC). Each internship led to a unique direction of research in areas of work highly relevant to the national labs. Without lab collaboration it would have been more difficult to recognize the significance of and to pursue this work. Whereas I have benefitted from some excellent HPC-related courses at UNM, there is a lot of knowledge in HPC that, unfortunately, isn't taught in any classes and that must be learned independently through professional presentations or conversations with lab scientists. Internships and collaboration with national labs has given me the opportunity to learn some of this knowledge and has provided projects to guide this learning.

Braxton Cuneo (braxton.s.cuneo@gmail.com
Degree in Progress: PhD, Computer Science, Oregon State University ✦ Advisor: Prof. Mike Bailey ✦ PSAAP: 2016-Present

Research Topic

On-GPU Asynchronous Scheduling for Monte Carlo Neutron Transport

Research Responsibilities

I work as a software researcher in the Center for Exascale Monte-Carlo Neutron Transport (CEMeNT). My research investigates methods of supporting programs with variable resource demands on graphics processing units (GPUs). Science and industry are increasingly relying upon the high processing throughput of GPUs, but GPUs achieve this high performance by optimizing for specific processing patterns – where threads in the same group take similar paths through a program.

Many applications, including Monte-Carlo Neutron Transport, can exhibit variable and practically unpredictable processing patterns. My research focuses on developing a framework that dynamically re-organizes the operations required by a program through an on-GPU asynchronous scheduler. By segmenting a program into a set of asynchronous functions, my framework can delay and re-assign processing so that threads in the same group take similar paths through the program. Through my framework, developers can focus upon the logic of their applications while the process of efficiently evaluating it on-GPU is handled automatically.

Benefits of PSAAP

Thanks to the Predictive Science Academic Alliance Program (PSAAP), I have been able to participate in the innovative work of CEMeNT, a group of some of the most fascinating people I have ever met. My involvement in this interdisciplinary, inter-institutional team of experts has exposed me to new areas of study which have shaped the path of my research for the better. With the resources and guidance provided by my research group, I feel well-prepared for working in professional, research-oriented settings. In addition, the network of professional relationships I have developed through this research group represents a powerful support network for my future research.

New Contacts, New Opportunities

Through my participation in the CEMeNT group, I had the opportunity to work at Lawrence Livermore National Laboratory (LLNL) over the Summers of 2021 and 2022, working with leading experts in radiation transport to improve the quality and performance of research code. Over the Summer of 2021, I was fortunate enough to work on the codebase of MERCURY, LLNL's next-generation radiation transport software, investigating optimizations or memory performance. In the following summer, I was able to contribute to the vectorization capabilities of RAJA, LLNL's high performance computing portability library. Through these work opportunities, I gained hands-on experience at a world-class research institution and helped advance the sum of human knowledge.

Isabella Gessman (gessman2@illinois.edu)
Degree in Progress: PhD, Mechanical Science and Engineering, University of Illinois at Urbana Champaign ✦ Advisors: Tonghun Lee and Greg Elliott
PSAAP: 2020-Present

Research Topic

Laser Diagnostics for Scramjet Experiments

Research Responsibilities

The Center for Exascale-enabled Scramjet Design (CEESD) is a collaboration of students, researchers, and professors from a broad range of disciplines developing the simulations, quantifying uncertainty, and providing experimental validation for carbon-based material implementation in a hypersonic combustion environment. These materials are inserted in the cavity of a scramjet flowpath and tested in the ACT-II facility that I run at Illinois.

Benefits of PSAAP

The Predictive Science Academic Alliance Program has provided a collaborative community with expertise in diverse fields. It has given me the opportunity to work with students and professors working on experiments, simulations, and computer science.

New Contacts, New Opportunities

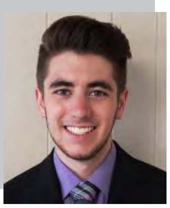
The program certainly has allowed me to work with others I would not have otherwise. The Center consists of both experimental and computational mechanical engineering students, computer science students forming the backbones of the computational tools, and aerospace students with a broad range of expertise from materials to fluid dynamics to laser diagnostics. The Center seems unique in how directly we experimentalists work with the simulation team. Communication is maintained throughout the entire Center to ensure coherence and understanding. These connections allow problems to be approached from different perspectives and collaboration across diverse disciplines.

National Laboratory Experience

Through CEESD, I completed an internship at Sandia National Laboratories (Sandia) in the Summer of 2022. This was a great experience and the best introduction to national laboratory research I could imagine. My internship responsibilities primarily consisted of taking absolute emission measurements to characterize the shock-heated gas in Sandia's High Temperature Shock Tube (HST). I worked closely under the mentorship of Kyle Daniel, Justin Wagner, and Kyle Lynch who provided direction and guidance for the experiments. The knowledge and experience I gained is continuing to help my PhD research, and I have chosen to continue as a year-round intern to facilitate continued collaboration. Future work will consist of connecting upcoming laser absorption experiments in the HST with closely-related experiments that will be carried out at Illinois in the ACT-II facility.

Samuel Lamont (samuel.lamont@colorado.edu)
Degree in Progress: PhD, Mechanical Engineering, University of Colorado Boulder ✦ Advisor: Dr. Franck Vernerey
PSAAP: 2021-Present

Research Topic



Mechanics of Soft Materials and Time-dependent Material Behavior

Research Responsibilities

My research responsibilities include developing numerical modeling strategies, performing validation and verification on simulations, experiments, and processing, and developing theoretical models for materials with complex response.

My focus in the Multi-disciplinary Simulation Center is developing simulation techniques to explicitly model the effects of processing conditions on our mock HE material. During manufacturing, a mixture of particulate matter and polymeric binder are pressed in a cylindrical die and exposed to high temperature (50°) and pressure (300 MPa) for one minute. This induces a myriad of complex mechanical behaviors including phase change (glassy transition), fracture, and bonding/debonding between particles and binder. To predict the behavior of this system, I am developing explicit particle-based strategies for modeling the polymeric binder in a way that integrates with the Discrete Element Method (DEM) commonly used for modeling granular systems. This would enable the ability to run largely scalable simulations of particle-polymer systems that resolve grain-level physics within an exascale computing workflow.

Benefits of PSAAP

I have benefitted from the Predictive Science Academic Alliance Program (PSAAP) by having the opportunity to develop not only my technical skills but also by getting to present and explain my work to a large Center. This extra practice of communication and team collaboration has been extremely useful and is probably the biggest advantage of PSAAP.

New Contacts, New Opportunities

My work in the CU Boulder Predictive Science Academic Alliance Program III (PSAAP III) has given me access to powerful High Performance Computing (HPC) resources and the opportunity to pursue the research that interests me within the context of the Center. Thanks to this program, I was selected for a summer internship at Sandia National Laboratories. There, I developed practical software development skills by working on a custom plugin for modeling viscoelasticity in dynamic polymers within the LAMMPS molecular dynamics codebase. This work excites me, as it enables direct investigation of the influence of small-scale physics on large, complex systems using the power of modern computational technology.

Mae Sementilli (maesemen@buffalo.edu)

Degree in Progress: PhD, Aerospace Engineering, University at Buffalo ✦ **Advisor:** Dr. James Chen ✦ **PSAAP:** 2020-Present

Research Topic

Volume of Fluid Simulation Development for Compressible, Multiphase Flow

Research Responsibilities

My responsibilities in the University at Buffalo's Center for Hybrid Rocket Exascale Simulation Technology (CHREST) include the development of scalable, multiphase flow solvers for the Center's software framework, Ablative Boundary Layers at the Exascale (ABLATE). My current research has been on developing a highly-parallelizable, compressible Volume of Fluid solver capable of capturing shear flow instability present at the fuel surface in hybrid rockets. Simulations of the fuel generated by this solver will be analyzed with a focus on understanding interface instability growth leading to droplet pinch off. Beyond development of the solver, I have been working with the verification and validation of these multiphase flow results, as well as performance testing on the Lawrence Livermore National Laboratory (LLNL) supercomputer, Quartz. Some of my future work would include the exploration of surface tension models as well as the integration of the multiphase solver with chemical reaction, phase change, and other modeling techniques for the overall goal of simulating a complete burn in a hybrid rocket motor.

Benefits of PSAAP

Being a part of the CHREST research Center has given me great relationships with students from other disciplines and the ability to work collaboratively on a groundbreaking project. I have expanded my network of faculty who have experience with multiphase flow simulation from whom I can seek advice on various aspects of my research. In addition to the connections at my institution, the PSAAP program has given me the opportunity to spend the summer at Los Alamos National Laboratory (LANL) for an internship and to make connections in the greater computational fluids community. I have been able to utilize the vast computing resources from LLNL in my research in testing multiphase fluid code.

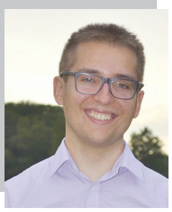
National Laboratory Experience

The internship experience I had at LANL this past summer has started connections with experts in the field who will be invaluable resources for technical advice moving forward. The advice that I received from my mentors in aspects that I had neglected in the development of my formulations enabled me to make important breakthroughs in my research. My mentors also gave me insight on what a career as a research scientist looks like. In addition, I forged relationships with potential advisors for future research, which could lead to career opportunities at the national laboratories.

Adam A. Sliwiak (asliwiak@mit.edu)

Degree in Progress: PhD, Computational Science and Engineering, Massachusetts Institute of Technology ✦ **Advisor:** Prof. Qiqi Wang

PSAAP: 2020-Present



Research Topic

Sensitivity Analysis of Chaotic Dynamical Systems

Research Responsibilities

Based on the theory of chaotic dynamical systems, I develop numerical methods enabling accurate prediction, control, and uncertainty quantification of chaotic models that are prevalent in turbulence and climate dynamics. Systems of this type are subject to the famous butterfly effect, i.e., exponential separation of any pair of nearby trajectories everywhere on the attractor. Consequently, the majority of popular algorithms, which rely on the propagation of the system's perturbations in time, blow-up exponentially fast making the analysis of such models extremely challenging. To overcome this difficulty, I extended the method known as the space-split sensitivity (S3) to high-dimensional systems. S3 had been rigorously derived based on the linear response theory and provides a set of provably converging and stable trajectory-following expressions that directly relate the input perturbation (e.g., imposed forcing, boundary condition, or geometric parameter) with the system's response (e.g., long-time averages of the user-defined objective function). I successfully applied the newly developed method to a number of chaotic systems, ranging from simple one-dimensional maps to equations describing turbulent fluid motion.

Benefits of PSAAP

I would like to emphasize that the Predictive Science Academic Alliance Program (PSAAP) provides an excellent opportunity to work with scientists and engineers from different disciplines and institutions which, in my opinion, is the greatest value of this research program. Our PSAAP project blends concepts and techniques from Applied Mathematics, Fluid Mechanics, and Software Engineering. Working in such an interdisciplinary environment did not only broaden my technical knowledge, but also improved my communication skills, my ability to handle multiple tasks simultaneously, and my ability to manage time efficiently.

National Laboratory Experience

During the Summer of 2022 as an intern at Sandia National Laboratories, I explored projection-based Reduced Order Modeling (ROM) techniques in the context of chaos. This uncharted territory is full of questions and challenges relevant to our PSAAP project. We concluded that the Galerkin-proper orthogonal decomposition (POD) method could potentially serve as a reliable tool in parametric studies of dynamical systems. Before this happens, however, we first must learn how to assess the quality of ROM solutions subject to the butterfly effect. Another fundamental question concerns potential extensions of the classical POD representation of multiscale models. We tackled some of these challenges by running several numerical experiments using both the Kuramoto-Sivashinsky and three-dimensional, compressible Navier-Stokes equations as test cases. This work established several interesting directions for future research in the field of data-driven methods.

Students

The Predictive Science Academic Alliance Program (PSAAP) is responsible for making my graduate studies a possibility. Simply put, without PSAAP, I would not have had the opportunity to pursue a PhD and a career in research, as I am entirely self-funded without any help from family or elsewhere. Beyond making my pursuits possible, participation in PSAAP has given me numerous opportunities.

Gerald Collom
University of New Mexico

The internship experience I had at LANL this past summer has started connections with experts in the field who will be invaluable resources for technical advice moving forward. The advice that I received from my mentors in aspects that I had neglected in the development of my formulations enabled me to make important breakthroughs in my research. My mentors also gave me insight on what a career as a research scientist looks like.

Mae Sementilli
University of Buffalo

Through CEESD, I completed an internship at Sandia National Laboratories (Sandia) in the Summer of 2022. This was a great experience and the best introduction to national laboratory research I could imagine. My internship responsibilities primarily consisted of taking absolute emission measurements to characterize the shock-heated gas in Sandia's High Temperature Shock Tube (HST). I worked closely under the mentorship of Kyle Daniel, Justin Wagner, and Kyle Lynch who provided direction and guidance for the experiments. The knowledge and experience I gained is continuing to help my PhD research, and I have chosen to continue as a year-round intern to facilitate continued collaboration.

Isabella Gessman
University of Illinois at Urbana Champaign

Minority Serving Institutions Partnership Program

The 30 Consortia of the Minority Serving Institutions Partnership Program and Tribal Education Partnership Program

American Indian Higher Education Consortium (AIHEC) | Lead: American Indian Higher Education Consortium | Sub-Recipients: Navajo Technical University, Salish Kootenai College, Turtle Mountain Community College, Cankdeska Cikana Community College, Bay Mills Community College | NSE Collaborators: KCNSS, SNL

The AIHEC consortium develops and offers advanced manufacturing academic programs at Tribal Colleges and Universities (TCUs), implements outreach and recruitment plans targeting both high school and college students, develops research, development, and manufacturing project opportunities at the Advanced Manufacturing Network Initiative (AMNI) TCUs, strengthens the engineering and technical career pathway for all TCU students, expands the TCU AMNI consortium, and coordinates with NNSA national laboratories on provisions of outreach, recruitment, and technical assistance resources to the TCUs.

National Security Enterprise (NSE) Collaborators

Partial DOE National Laboratories List

ANL	Argonne National Laboratory
BNL	Brookhaven National Laboratory
INL	Idaho National Laboratory
KCNSC	Kansas City National Security Campus
LANL	Los Alamos National Laboratory
LLNL	Lawrence Livermore National Laboratory
NNSS	Nevada National Security Site
NREL	National Renewable Energy Laboratory
ORNL	Oak Ridge National Laboratory
PNNL	Pacific Northwest National Laboratory
SNL	Sandia National Laboratories
SRNL	Savannah River National Laboratory
Y-12	Y-12 Security Complex

Advanced Sensors Technologies for Applications in Electrical Engineering - Research And Innovation Excellence Consortium (ASTERIX) | Lead: Florida International University | Sub-Recipients: Florida A&M University, Miami Dade College NSE Collaborators: KCNSC, LANL, Y-12

The ASTERIX consortium focuses on advanced sensors and systems to develop highly-sensitive, multiplexed ion-traps integrated with getter-based vacuum systems and radiation-hardened electronics packaged for harsh environments using laminating and three-dimensional (3D) printing technologies. Through this advanced research, the ASTERIX Consortium trains students on nuclear safety sensors and systems and uses this training to build a sustainable pipeline of talented, diverse, engineering students ready to enter the science, technology, engineering, and mathematics (STEM) workforce of the Department of Energy/National Nuclear Security Administration (DOE/NNSA).

Advanced Synergistic Program for Indigenous Research In Engineering (ASPIRE) | Lead: Turtle Mountain Community College | Sub-Recipient: United Tribes Technical College | NSE Collaborators: KCNSC, LANL, SNL

The ASPIRE consortium implements outreach activities for students in grades 6-12, enhances the engineering curriculum at all colleges, improves technical capacity, advances the technical knowledge of engineering students, and offers support for students who transfer to a four-year engineering program. The tribal colleges recruit students into engineering programs, offer mechanical and electrical engineering courses, and provide experience with the national laboratories.

Additive Manufacturing Post Processing Partnership (AMP3) | Lead: University of the District of Columbia | Sub-Recipients: Howard University, Morgan State University | NSE Collaborators: KCNSC, ORNL, Y-12

The Consortium for Additive Manufacturing Post Processing Partnership's (AMP3) objectives are to recruit and attract undergraduate, graduate, and post-doctoral trainees who matriculate into STEM careers with a concentration in Additive Manufacturing (AM); to create experiences for trainees in AM and associated fields through coursework, extracurricular opportunities, and internships; to leverage synergies between Historically Black Colleges and Universities (HBCUs) that enable cutting-edge research collaborations in AM; and to create partnerships with NNSA labs and plants that advance HBCU research capacity in AM, providing a pathway for students and post-doctoral employment.

Application of Artificial Intelligence to Cybersecurity for Protecting National Critical Infrastructure (CONCISE) | Lead: University of Texas at San Antonio | Sub-Recipients: North Carolina A&T State University, Savannah State University, University of Nevada, Las Vegas | NSE Collaborator: NNSS

CONCISE has three objectives: to enhance the Minority Serving Institutions' (MSIs) Industrial Internet of Things (IIoT) cybersecurity education capacity, to enhance MSIs' IIoT cybersecurity research capacity, and to create and sustain a DOE/NNSA cybersecurity workforce recruitment pipeline. The project will develop a range of prototype systems, including artificial intelligence-based (AI-based) IIoT intrusion detection systems, AI-based malware detectors, and blockchain-based automated IIoT cybersecurity management systems.

Attract, Educate, Train, and Retain Native American and Minority Students in Nuclear & Related Sciences (AETERNAMS) | Lead: Nueta Hidatsa Sahnish College | Sub-Recipient: Alcorn State University | NSE Collaborator: LANL

The goals of AETERNAMS are to attract, educate, train, and retain a significant number of Native American and minority students into STEM and related fields; introduce STEM concepts to students and local high school teachers; provide research opportunities to high school students; help students to gain research experience at partnering universities and national laboratories; and professionally prepare students for STEM careers.

Consortium of Advanced Additive Manufacturing Research And Education for Energy Related Systems (CA2REERS)

| Lead: The University of Texas-Rio Grande Valley | Sub-Recipients: University of Arizona, University of Texas at San Antonio
NSE Collaborators: LANL, ORNL

The goal of CA2REERs is to expose, recruit, engage, and train students from underrepresented groups for a career in Advanced Manufacturing for Energy, following a collaborative approach by a team of investigators from three MSI institutions and two DOE laboratories. The long-term vision of the consortium is to cultivate an innovation-driven manufacturing education ecosystem for Energy Innovation with programs designed to recruit young talent and prepare them with a solid education and real-life experiences in energy innovation and advanced manufacturing technologies.

Consortium Enabling In- and Ex-Situ-Quality Control of Additive Manufacturing (QCAM)

| Lead: New Mexico State University | Sub-Recipients: Navajo Technical University, Prairie View A&M University | NSE Collaborators: KCNSC, LANL, ORNL

The main goal of QCAM is to establish a sustainable pipeline of students from underrepresented minorities to the NNSA laboratories who specialize in new methods of additive manufacturing (AM) and non-destructive testing (NDT) that mitigate traditional obstacles to these fields.

Consortium for High Energy Density Science 2.0 (CfHEDS-2)

| Lead: Florida A&M University | Sub-Recipients: Morehouse College, University of California-Merced | NSE Collaborator: LLNL

The goal of CfHEDS-2 is to sustain the pipeline that was been created by the previous award by enabling MSIs to develop scientists who are well prepared to work in the NNSA-critical field of high energy density science (HEDS). Two major thrusts are being pursued: 1) education, outreach, and internship programs and 2) scientific objectives in HEDS that increase the understanding of the effects of a dense plasma on plasma bound states both experimentally and theoretically, modeling the transition from cold solid matter to HED plasmas; and studying time-resolved, X-ray spectroscopy on electron-ion temperature relaxation.

Consortium for Laser-Based Analysis of Nuclear And Environmental Materials (LANEM)

| Lead: Florida A&M University | Sub-Recipients: Alabama State University, Delaware State University | NSE Collaborator: Y-12

LANEM has two primary objectives: 1) strengthen the network of the five partners by developing interdisciplinary, collaborative projects aimed at increasing the precision and enhancing the accuracy of the detection and identification of materials by combining laser-based technologies, such as laser-induced breakdown spectroscopy (LIBS) and fluorescence imaging, with novel, analytical tools and modeling; and 2) broaden and increase opportunities for diversity in the workforce in NNSA research areas by engaging STEM students, postdoctoral fellows, and faculty members who will participate in comprehensive training programs and internships in the LANEM academic institutions and national laboratories.

Consortium for Research and Education in Materials Science and Photonics Engineering (NoVEL)

| Lead: Norfolk State University | Sub-Recipients: Elizabeth City State University, Virginia State University | NSE Collaborator: LLNL

The key objectives NoVEL are to 1) strengthen the research and education capabilities in the research areas of materials science and photonics; 2) recruit and prepare talented students to excel in STEM by providing them with career-readiness skills, fundamental knowledge, practical experience, and training through applicable cutting-edge research projects, capacity building, and experiential learning; and 3) enlarge the fundamental scientific and technical knowledge and resource base in the areas of materials science and photonics (such as controlling light-matter interaction with metamaterials). These objectives are being achieved via formal and informal education and training, student internships, and involving students in the cutting-edge research.

Consortium for Research and Education In Power and Energy Systems (CREPES)

| Lead: Florida International University | Sub-Recipients: Alabama A&M University, University of Texas at El Paso | NSE Collaborators: LLNL, SNL

CREPES is structured to excel in STEM by carrying out transformative and applicable research with practical experience and training in the area of Electrical Engineering, with emphasis on Electric Power and Energy Systems Engineering, Nuclear Engineering, and related Cyber and Information Security issues. CREPES will educate the next generation of a diverse Energy Systems workforce at MSIs by delivering strong analytical skills and increased interests in advanced research relevant to the NNSA.

Consortium for Nuclear Security Advanced Manufacturing Enhanced by Machine Learning (NSAM-ML)

| Lead: North Carolina Central University | Sub-Recipients: Elizabeth City State University, Southern University Baton Rouge | NSE Collaborators: LANL, SNL

NSAM-ML has four main objectives: 1) build a large research body capable of solving difficult problems relative to advanced manufacturing and material fabrication; 2) solve extremely challenging materials processing problems to enable the production of materials that are efficient for nuclear safety and security; 3) use Machine Learning to extract hidden information on materials that otherwise hinder advanced manufacturing; and 4) build capacity that enables partnering universities to create an NNSA research pipeline. The project aims at generating new types of manufacturing methods and attaining detailed knowledge of processes at the molecular and atomic levels.

Consortium Hybrid Resilient Energy Systems (CHRES) | Lead: Universidad Ana G. Méndez-Gurabo | Sub-Recipients: University of New Mexico, University of Puerto Rico-Mayague, University of Texas at El Paso | NSE Collaborators: LLNL, NREL, SNL

CHRES activities are to (1) provide high school students with a college educational experience where they are exposed to engineering topics, with a special emphasis in resilient energy systems; (2) provide high school students with a college research experience where they are exposed to resilient energy systems topics; (3) integrate undergraduate and graduate students into the research efforts at the universities and national laboratories; (4) integrate Hispanic serving institutions' (HSIs) research and education with national laboratories' efforts; (5) organize dissemination activities to present consortium activities to peers and the community; (6) enable engineering and technology research in STEM undergraduate and graduate education; and (7) enable collaboration among the academic institutions, the national laboratories, and the public and private sectors.

Consortium on Nuclear Security Technologies (CONNECT) | Lead: University of Texas at San Antonio | Sub-Recipients: St. Mary's University, University of Nevada, Las Vegas | NSE Collaborators: ANL, PNNL

The overarching goal of CONNECT is to educate and train the best, next-generation professionals with strong backgrounds in nuclear science, fissionable fuels fabrication and processing, nuclear materials characterization, nuclear forensic signatures, nuclear technology, and data and visual analytics each collaboratively brought to bear on expanding the innovation envelope of nuclear security.

Consortium for Education and Research In Electronics for Extreme Environments (E3C) | Lead: University of Texas at El Paso | Sub-Recipients: North Carolina A&T State University, University of New Mexico | NSE Collaborators: KCNSC, LANL, SNL

The Consortium aims to offer the next-generation of underrepresented minority (URM) electrical engineers a strong background in electronics for extreme environments.

Enabling Native Researchers and Graduate Engineering (ENRGE) | Lead: Navajo Technical University | Sub-Recipients: Alabama A&M University, Florida International University | NSE Collaborators: INL, NREL

The goal of the ENRGE Consortium is to increase the number of Native American researchers with undergraduate and graduate education in engineering disciplines by building the first masters degree and doctoral degree programs in engineering at tribal universities through four objectives: 1) enhance the undergraduate engineering programs at Navajo Technical University, 2) develop robust graduate programs in engineering with concentrations in Electrical Engineering, Mechanical Engineering, Computer Engineering, Nuclear Engineering and Energy Systems, and Industrial Engineering and Advanced Manufacturing, 3) build sustainable collaboration networks with DOE/NNSA facilities and researchers, and 4) build hands-on training and research capabilities in Advanced Energy Systems and Nuclear Safety.

Energy Sciences: Experimental and Modeling Consortium (ESEM) | Lead: Prairie View A&M University | Sub-Recipients: InterAmerican University, Puerto Rico San German, Morehouse College, Tennessee State University | NSE Collaborators: LANL, PNNL

ESEM partners carry out collaborative research activities specifically designed to build research skills and student confidence; offer workshops presented by consortium members, industry partners and DOE laboratories; acquire and upgrade common research capacity to provide cross-board validation and promote inclusive training and research environments; provide training to better prepare MSI participants and increase their competitiveness to be hired in the workforce; continue successful execution of the research and training plan and the realization of milestones and deliverables.

Growing Stems Consortium: Training The Next Generation of Engineers for the DOE/NNSA Workforce (GSC) | Lead: Texas Tech University | Sub-Recipients: Amarillo College, New Mexico Institute of Mining and Technology, University of California–Merced | NSE Collaborators: LANL, SNL, Y-12

GSC objectives target four learning environments designed to grow the number of minority students earning engineering degrees and transitioning into the DOE/NNSA workforce: 1) Research-Centered Student Training on DOE/NNSA collaborative research projects for undergraduate and graduate student participants; 2) Student Induction into the DOE/NNSA workforce through internships; 3) Student Recruitment and Education with an emphasis on technical foundational courses for technician training certifications and a wide array of professional development activities; and 4) Engineering Outreach impacting the next-generation of minority students earning STEM degrees.

Integrated Additive Manufacturing – Establishing Minority Pathways: Opportunities for Workforce-Development In Energy Research and Education (IAM-EMPOWEREd) | Lead: Florida A&M University | Sub-Recipients: Benedict College, University of Texas–Rio Grande Valley | NSE Collaborators: KCNSC, LANL, Y-12

The primary aim of IAM-EMPOWEREd is to utilize state-of-the-art Direct Writing (DW) and three-dimensional digital printing (3DP) research for integration of complex and multifunctional material device fabrication. The target is to advance manufacturing research and training across additive-processed ceramics, polymers, composites, and metals.

Indigenous Mutual Partnership to Advance Cybersecurity Technology (IMPACT) | Lead: Turtle Mountain Community College | Sub-Recipients: Sitting Bull College, Stone Child College | NSE Collaborators: KCNSC, SNL

The goal of IMPACT is to strengthen and expand STEM and cybersecurity education and research at three Tribal Colleges, preparing a highly-qualified, next-generation workforce and increasing the flow of American Indian/Alaska Native students into cybersecurity careers throughout the NSE to meet present and future security demands.

Microelectronics & Materials Engineering Education for Nuclear and Cyber Security (MEMENCYS) | Lead: University of California–Riverside | Sub-Recipient: University of California–Irvine | NSE Collaborator: SNL

The goal of MEMENCYS is to create a diverse, educational pipeline in the field of microelectronics where participants are inspired to secure future careers in NSE laboratories through exposure to research with Consortium partners. The objectives to achieving this goal are to: 1) support education at all levels to maximize participant retention and to promote diversity; 2) educate and train students in areas of interest to the NNSA; and 3) investigate unanswered questions in the modification and manipulation of electronic materials and quantum devices from ion irradiation.

Nuclear Security Science and Technology Consortium (NSSTC) | Lead: University of Nevada–Las Vegas | Sub-Recipients: University of Illinois at Chicago, University of New Mexico | NSE Collaborators: ANL, LANL, NNSS

The main goal of NSSTC is to develop the next-generation, world-class, STEM workforce to meet national security demands, strengthening key science, technology, and engineering capabilities to support the NNSA's vital mission. Consortium members address overarching themes within the topical research area of nuclear security. The sub-topic areas include radiation detection systems for nuclear security applications, nuclear forensics, X-ray fluorescence for radionuclide and actinide detection, and remote sensing of radiological and nuclear materials.

Partnership for Advanced Manufacturing Education and Research (PAMER) | Lead: Navajo Technical University | Sub-Recipients: Nebraska Indian Community College, Southwestern Indian Polytechnic Institute, University of Texas at El Paso | NSE Collaborators: LANL, ORNL, SNL

PAMER focuses on providing opportunities for American Indian student research internships, research skills training, research collaboration, and increasing public awareness of DOE/NNSA scientific activities. Activities include K-12 outreach, new courses, seminars and workshops, annual meetings, guest speakers and lectures, tours of the national laboratories, STEM demonstrations, student co-advising on projects including capstone projects, student internship, student research training and experiences, joint TCUs-NNSA advanced manufacturing research projects, NSE presence at PAMER schools' career fairs, websites, and social media.

Partnership for Proactive Cybersecurity Training (PACT) | Lead: The University of Arizona | Sub-Recipients: Howard University, Navajo Technical University | NSE Collaborator: ANL

PACT's goals are to: 1) establish a comprehensive, cybersecurity science agenda that provides the theoretical foundation to: (a) use data analytics and machine learning science to accurately and precisely quantify and characterize "normal" operations of cyber systems and services; (b) model and quantify the risks and impacts of vulnerabilities and attacks on cyber systems, (c) develop data-driven, cybersecurity and forensic modeling, analysis, and prediction; and (d) design and analyze innovative detection and protection techniques; 2) validate and demonstrate the usefulness of the cybersecurity solutions on large-scale case studies; and 3) integrate the Consortium's research projects with established cybersecurity educational and training programs. The Consortium will recruit underrepresented minority students for involvement in research projects, cybersecurity summer training and mentoring camps, and internship programs.

Partnership for Radiation Studies (PaRS) | Lead: Alabama A&M University | Sub-Recipient: Fisk University | NSE Collaborators: PNNL, SRNL

The objectives of the PaRS Consortium is to create a sustainable and scalable pipeline for minority students. Student recruitment and education opportunities include recruitment activities through workshops and seminars at K-12, regional community colleges, and member MSIs; research and student training; and outreach to transition student participants into DOE/NNSA national laboratories through joint student advisement, joint research, and co-op opportunities that lead to employment after graduation.

Partnership for Research and Education Consortium in Ceramics and Polymers 2.0 (PRE-CCAP-2) | Lead: University of Texas at El Paso | Sub-Recipients: Florida International University, Tennessee State University | NSE Collaborators: KCNSC, LANL

PRE-CCAP-2 is a 5-year renewal to expand and sustain a pipeline of the diverse, highly-trained workforce and a community of technical peers with a focus in Materials Science. Its expanded project objectives are to grow and sustain the student pipeline, establish Interdisciplinary Research Groups (IRGs) for joint success and increased STEM research capacity, grow and assess the impact and visibility of a long-term educational and outreach plan, and sustain the research and education pipeline beyond the expiration of the grant.

The Rio Grande Consortium for Advanced Research on Exascale Simulation (GRANDE CARES)

| Lead: University of New Mexico | Sub-Recipients: New Mexico Institute of Mining and Technology, New Mexico State University, Prairie View A&M University, University of Texas at El Paso | NSE Collaborator: SNL

The Rio Grande CARES team aims to bolster an in-depth understanding of multiphysics concepts from multiple disciplines and crosscutting technologies through research thrusts and an innovative curriculum. The consortium's objectives are to 1) formulate, validate, and implement advanced computational tools operating efficiently with extremely large databases for system-level predictions; 2) develop high-fidelity, multiphysics, computational approaches; and 3) deploy leading-edge, computational tools from SNL through integrative curriculum changes to develop a sustainable approach to workforce needs.

Scholarly Partnership in Nuclear Security (SPINS) | Lead: Alabama A&M University | Sub-Recipients: Navajo Technical University, University of Puerto Rico–Rio Piedras | NSE Collaborators: BNL, LANL, SRNL

The vision of the Scholarly Partnership in Nuclear Security (SPINS) is to enhance the development of the next-generation technical workforce for the NNSA through active-learning-based education and collaborative state-of-the-art research in nuclear security, radiation detection systems, and nuclear nonproliferation that engage and broaden the participation of underrepresented minority men and women (specifically African Americans, Hispanics, and Native Americans).

Successful Training and Effective Pipelines to National Laboratories with STEM Core (STEP2NLS)

| Lead: North Carolina A&T State University | Sub-Recipients: Growth Sector Company, Navajo Technical University, New Mexico State University | NSE Collaborators: LLNL, SNL, Y-12

The STEP2NLs Consortium works to deliver comprehensive and intensive pathways that introduces students to STEM opportunities; provides accelerated math skills development; creates awareness of jobs in the computer-science and cybersecurity sectors; incorporates needed social, academic, and financial support; offers paid-internship and research opportunities; and connects students to 2- and 4-year degree pathways at partner educational institutions.

Bryan Franzoni (franzb1@unlv.nevada.edu)
Degree in Progress: BS, Mathematics, University of Nevada, Las Vegas ✦ Advisors: Dr. Evan Scott and Dr. Michael Weller ✦ MSIPP: 2022-Present

Research Topic

Improving the XTR Software Code and Analyzing Optical Transition Radiation Beam Particle Images

Research Responsibilities

I joined the Mission Support and Test Services, Inc. as a summer intern in FY 2022 to work with Dr. Evan Scott (Senior Scientist) with the primary objectives of improving the XTR software code used for tuning the magnets of the linear induction accelerator and analyzing Optical Transition Radiation (OTR) beam particle images to find their center and radius. The tools used are IDL and Linux (for the XTR project) and Python (for the OTR project).

Benefits of MSIPP

The Minority Serving Institutions Partnership Program (MSIPP) has provided me the opportunity to help current research by analyzing the XTR beam envelope code and learn its archaic language, i.e., IDL. When I got a hang of the basic syntax, I started fixing the issues that nagged my mentors the most: directory and error handling. Luckily, it only took a few weeks to resolve those issues, and it was enough time to move onto more demanding tasks.

For the remainder of my time, I then used a python IDE called Spyder to write a program tasked with fitting Gaussian curves to arrays of images, which helped extract all the information my mentors needed to verify. This enabled me to improve my python skills by using popular statistical packages such as Numpy and Scipy, which are very useful skills to learn for any research setting.

In short, the MSIPP-CONCISE program gave me an unencumbered 12 weeks of time in an exciting fast-paced environment. My mentors were always there to answer any questions I had, and gave me guidance whenever I got stuck, which ultimately led to the success of both projects. Thus, I would recommend giving this incredible opportunity a shot to anyone considering signing up for the program.

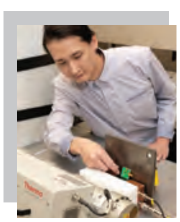
What Students Considering MSIPP Should Know

MSIPP-CONCISE provides aspiring undergraduate and graduate students work opportunities on projects related to national security. It offers a perfect technical conduit to transition from academia to applied industrial / commercial research. It is a flexible training program that prepares students for scientific industries.

Charles Han (HanCD_EX@nv.doe.gov)
Degree in Progress: MSE, Mechanical Engineering, Fall 2024 (expected), University of Nevada, Las Vegas ✦ MSIPP: 2021-Present

Research Topic

Monte Carlo Simulation with GEANT4 for Novel Radiation Detection Materials



Research Responsibilities

I joined the Mission Support and Test Services, Inc. as a summer intern in FY 2022 to work with Dr. Andrew Jesse Green, Senior Principal Scientist, with the primary objectives of performing Monte Carlo simulations using GEANT4 for novel radiation detection of materials like perovskite crystals and single crystal chemical vapor deposition (scCVD) diamond.

Benefits of MSIPP

The Minority Serving Institutions Partnership Program (MSIPP) – Nuclear Security Science and Technology Consortium (NSSTC) has provided me with the opportunity to focus on my research on material informatics for 12 unencumbered weeks in a science environment at the Nevada National Security Site (NNSS) and to learn from practicing physicists and material scientists.

New Contacts, New Opportunities

MSIPP provided me with ample opportunities to work with my immediate mentor, Dr. Green, and the project manager, Dr. Amber Guckes, and also with other interns at NNSS from MSIPP programs.

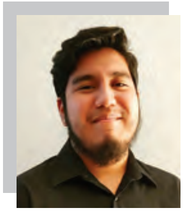
I spent 12 weeks at the North Las Vegas campus of NNSS, where I worked with experienced personnel who routinely perform nuclear-security-related physics experiments under extreme physical conditions (high temperature, high pressure). Understanding physical conditions like phase transition, stability, and structural details of materials under these extreme conditions are very important. My research contributed to this area by characterizing the detector response functions for gamma-ray and neutron radiation. The opportunity to gain unique experience from one of the premier nuclear security organizations has better prepared me to land highly specialized employment outside of the academic environment.

MSIPP Influence on Research Area or University

By choosing the subject topic, I was able to support the NNSS Site Directed Research and Development (SDRD) project. The research topic was mutually beneficial both for me and for NNSS.

Kevin Lugo (kevinr11301@gmail.com)

Degree in Progress: BS, Computer Science, University of Nevada, Las Vegas ✦ Mentor: Dr. Yoohwan Kim ✦ MSIPP: 2020-Present



Research Topic

Tabletop Exercise and Exercise 22 – Attack Framework

Research Responsibilities

I joined Mission Support and Test Services, Inc. as a summer intern in FY 2022 to work with Jay Chotimal, Bill Bixby, and Debbie Davies from the Special Technologies Laboratory (STL) in Santa Barbara, CA. STL is part of the Nevada National Security Site (NNSS), and I was able to work with STL from the North Las Vegas Complex of NNSS. I was assigned to the Tabletop Exercise and Exercise 22 – Attack Framework projects. The objectives of the Tabletop Exercise were to identify necessary roles and responsibilities to properly mitigate risks and vulnerabilities associated with eight different scenarios in a supervisory control and data acquisition (SCADA) and operational technology (OT) environment. The objective of the Exercise 22 – Attack Framework project was to develop an attack matrix on programmable logic controllers (PLCs) to construct a viable attack path and to validate the current Incident Response Plan.

Benefits of MSIPP

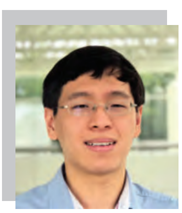
The Minority Serving Institutions Partnership Program (MSIPP) – Consortium On National Critical Infrastructure SEcurity (CONCISE) has provided me with the opportunity to gain awareness of and to develop research and interpersonal skills in operational technology and security. I already had SCADA/OT-related experience and knowledge of the associated high level programming languages. My education and laboratory experiences from UNLV were very suitable to the internship opportunities at the NNSS through the MSIPP-CONCISE internship, and I was encouraged and invited to join every meeting throughout this project. At any time, I was able to provide my own thoughts and ideas and learn the direction the overall team was taking. The Tabletop Exercise was scheduled to take place in mid-August 2022, and I was tasked with creating a presentation that would help facilitators lead the discussion. A physical test based off of this tabletop exercise was scheduled to take place late September 2022, and my assignment for my internship was to create an attack that could be implemented during red-teaming a simulated environment.

What Students Considering MSIPP Should Know

MSIPP-CONCISE provides aspiring undergraduate and graduate students opportunities to work on national security-related work. It is a flexible training program that prepares students for science-forward industries and is an excellent opportunity to prepare a student to transition from an academic environment to industrial or commercially-applied research.

Brandon Ma (bma@eagles.nccu.edu)

Degree: BS, Computer Science and Business, Computational Science, North Carolina Central University ✦ Mentor: Ember Sikorski, Sandia National Laboratories ✦ MSIPP: 2021-Present



Research Topic

Contribution to Development of Carbon Nanotube Database

Research Responsibilities

My research responsibilities were to conduct independent research on carbon nanotubes (CNTs), machine learning in relation to CNTs, and executing tasks given by my research advisors and team members. These included preparing data for processing, post-processing the data, writing up reports or papers, and assisting other team members in various tasks.

Benefits of MSIPP

Through the Minority Serving Institutions Partnership Program (MSIPP), I have been able to learn a number of topics outside of my usual field of study and have had the opportunity to work on a wide variety of software tools. These include Python, R language, Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), OVITO, Linux, and a few other software applications not available to the general public. My biggest achievement has been the creation of an automation script using Python at Sandia National Laboratories (Sandia) to streamline the data preparation process.

New Contacts, New Opportunities

MSIPP provides connections and offers a wide range of opportunities for students. In my case, prior to joining Sandia, I worked with a research team at NCCU which allowed me to better prepare for my summer internship. MSIPP did not influence my choice of research area or university, as I simply happened upon MSIPP by chance. However, for those of you who are interested in forming connections and being exposed to great opportunities such as internships or permanent jobs at Sandia or other national laboratories, MSIPP is a prospect that you should consider. MSIPP allowed me to work with researchers in the field of material science which is a research area to which I would not have been exposed without MSIPP. Whereas material science, physics, and chemistry are not my field of study, there are some overlaps between those fields and computer science. I have been exposed to the intertwining aspects of these fields mainly through software applications and tools, machine learning, and automation.

We were able to work on automation scripts independently but also were able to receive assistance by experts at Sandia when we needed help. This helped tremendously my knowledge and skills in Python programming. I also had the opportunity to learn about the research topics of other scientists and engineers at Sandia and even got a chance to work with a few software applications developed by Sandia. It would be an understatement to say only that this internship has benefitted my future career. The skills, knowledge, and experience I've gained from the internship have expanded my life choices.

Nixon Washington Ogoi (nogoi@eagles.nccu.edu)
Degree in Progress: BS, Physics, North Carolina Central University ✦ Advisor: Prof. Abdennaceur Karoui ✦ MSIPP: 2022-Present

Research Topic

- *Carbon Nanotube Mechanical Properties Using Molecular Dynamics and Development of Database for Machine Learning*
- *Hyper-doping of Silicon by Ion Implantation to Enable Infrared Absorption of Silicon*

Research Responsibilities

I have participated in two research projects of the Consortium for Nuclear Security Advanced Manufacturing by Machine Learning (NSAM-ML). These research projects are carbon nanotubes (CNT) mechanical properties in elastic and plastic regimes using large-scale, molecular dynamics (MD) calculations of tensile stress on CNTs and the development of a database for CNTs for material engineers developing new materials. I participated in data collection and analysis to draw meaningful conclusions on a wide range of CNTs. I have presented my research findings at conferences and in academic settings.

I had the opportunity to work as an intern at Los Alamos National Laboratory (LANL) where I performed simulations using the computer codes, SRIM and GEANT4, to design ion implantation experiments. I collaborated with a diverse team of researchers in designing and troubleshooting experiments and conducted experiments aligned with the mission priorities of the National Nuclear Security Administration (NNSA). Additionally, I conceptualized and implemented a cataloging system for over 900 parts deployed in equipment service.

Benefits of MSIPP

The Minority Serving Institutions Partnership Program (MSIPP) enabled me to explore research in physics and materials science at a deeper level than I would have been able to in a traditional classroom setting or in a typical undergraduate research experience. Through the opportunities offered by MSIPP, I was able to focus on research about which I am passionate. During my time working with NSAM-ML and as an intern at LANL, I have learned considerable technical skills that I never would have learned in the undergraduate, academic setting. MSIPP also has given me the opportunity to engage with top professionals at LANL and at Sandia National Laboratories (SNL).

What Students Considering MSIPP Should Know

MSIPP is an excellent program for students interested in science, technology, engineering, and mathematics and for those considering a career at one of the NNSA national laboratories. The opportunities offered through MSIPP are unmatched by any program of which I am aware.

LaSheena Ramone (lramone@sandia.gov)
Degree in Progress: MS, Computer Engineering, University of New Mexico ✦ MSIPP: 2021-Present

Research Topic

Higher Accuracy Separation Package Diode Tester

Research Responsibilities

During the summer of 2021, I was introduced to inertial clusters or inertial measuring units (IMU). The organization to which I was assigned needed a faster test setup for screening the diodes that are employed in the Higher Accuracy Separation Package (HASP) units on a reentry vehicle system. I was tasked to automate a diode screening tester using LabVIEW or LabVIEW NXG software. I worked my internship remotely, and the work required me to have test equipment, including power supplies and multimeters on hand. I gained valuable LabVIEW knowledge which allowed me to further my expertise in current LabVIEW projects outside of the MSIPP program.

Benefits of MSIPP

The MSIPP program introduced me to Sandia National Laboratories (Sandia). It helped me get my foot in the door, helped me to flourish, and helped me start my career at Sandia. My manager and mentors provided pep talks which were helpful. Additionally, my manager introduced me to other people with backgrounds similar to mine. We had presentations and discussions. These interactions helped instill the notion that if they can make it here, I can too. Seeing others like me at Sandia gave me more confidence that I belonged and inspired me. In simple terms, they were confidence boosters. Talking about my research with other professionals helped me improve my presentation skills for work and for school. Most importantly, I've been able to discover and develop a part of myself that I had not seen before. This part is going out and talking to people, asking for help when needed, and just being more comfortable overall. The MSIPP program at Sandia helped me grow as a person, a student, and a worker.

What Students Considering MSIPP Should Know

There are many opportunities out there. Please go out and find them. Ask questions. If one person doesn't know the answers, it is likely that another person will know them. When you get emails that say "Apply Here" for this summer internship, or if someone asks you to apply to a particular position, do it. Take advantage of all opportunities. When joining the MSIPP, take full advantage of what the program has to offer—get to know your managers, get to know your peer support, and get to know the general work environment. If you're feeling discouraged for whatever reason or if it seems scary, take a leap of faith. It could be life changing. Sandia and MSIPP were very helpful to me.

Geronimo Robles (geronimo.robles@utsa.edu)
Degree in Progress: PhD, Physics, Nuclear Fuel Materials, University of Texas at San Antonio ✦ **MSIPP:** 2019-Present

Research Topic

Synthesis of Fuel Cycle Materials

Research Responsibilities

My research includes material synthesis, material characterization, and data analysis for our research group at the University of Texas at San Antonio (UTSA) , national laboratory partners, and other university collaborators. I plan and run experiments, perform data analysis, and write publications about my proposed dissertation work related to the synthesis of fuel cycle materials. I prepare and submit speaker presentations and posters for academic conferences. I mentor undergraduate students by providing laboratory training and guidance about experimental plans and data analysis

Benefits of MSIPP

MSIPP has provided me the opportunity not only to pursue a course of study in nuclear material physics but also a pathway to a career. Without MSIPP I would not have any role models or examples to follow to see what success looks like in this field. Without MSIPP the completion of my degree would have required substantial additional time due to a need to work outside of my research in order to cover costs. This likely would have precluded my ability to work with the national laboratories. Most importantly, MSIPP facilitated introductions to experts in my field of research, especially at the national laboratories.

National Laboratory Experience

I returned to Los Alamos National Laboratory (LANL) in the Summer of 2022 for an internship that allowed me to further my dissertation work. My internship work was focused around completing the requirements for my qualifying exams including the fabrication, characterization, and testing of advanced nuclear fuels. At LANL, I was able to refine my experimental skills especially in the areas of arc melting, scanning electron microscopy and X-ray diffractometry sample preparation and analysis, and high temperature oxidation testing of uranium-bearing materials first acquired at and in collaboration with UTSA. There I produced materials by powder metallurgy and conventional pellet sintering both of which are skills and procedures not available at my university. The fuels being produced are uranium-silicide and uranium-boride composites. I was selected as a Seaborg Institute Summer Graduate Fellow and won an Outstanding Presentation award at the student symposium for some of the first results of my work. I then was offered and accepted the opportunity to remain at LANL as a full-time graduate assistant allowing me to complete my dissertation with my university tuition funded by the Consortium on Nuclear Security Technologies (CONNECT) and my research and employment funded by the Seaborg Institute and a Nuclear Thermal Propulsion (NTP) project.

Uttam Bhandari (ubhand2@lsu.edu)
Degree in Progress: PhD, Engineering Science, Louisiana State University ✦ **MSIPP:** 2020-Present

Research Topic

Designing Refractory, High-entropy Alloys using Machine Learning

Research Responsibilities

I am a PhD candidate co-supervised by Professor Yang, a co-principal investigator for the Consortium for the Nuclear Security Advanced Manufacturing enhanced by Machine Learning (NSAM-ML). My work for the Consortium is focused on research related to machine learning methods and density functional theory to predict the mechanical and thermal properties of refractory, high-entropy alloys (RHEAs). We perform experimental syntheses of RHEAs and characterize them using scanning electron microscropy (SEM) and transmission electron microscopy (TEM), including measuring their mechanical properties. Further, we investigate RHEAs by ion irradiation damage for their potential application as structural materials for next-generation fission and fusion reactors.

Benefits of MSIPP

My masters degree in computer science and physics at Southern University A&M College contributed to my acceptance into the Minority Serving Institutions Partnership Program (MSIPP). My continuing collaboration with Southern University A&M College and MSIPP helped me to gain an internship at Los Alamos National Laboratory (LANL). At LANL, I worked on ion implantation in two-dimensional materials, thin film materials, and alloys. During the internship I was able to attend research workshops and technical talks and to meet with high-caliber researchers. These experiences allowed me to better develop my research problem-solving skills.

National Laboratory Experience

Through MSIPP, I was able to participate in an internship at LANL that began in September 2022. MSIPP covers all of my travel and living expenses while at LANL which is a huge factor. Without this support, I would not be able to take advantage of an internship opportunity. While at LANL, I designed high-entropy alloys using machine learning methods and, then, synthesized them at my home institution. These types of materials are useful for nuclear technologies. They can increase the toughness of nuclear infrastructure and, therefore, can enhance nuclear safety.

As my internship continues, I will perform irradiation test of the alloy samples at LANL under the mentorship of LANL scientists. These tests will help in finding new, possible applications of RHEAs for various sectors such as the aerospace industry, nuclear reactors, and the motor industry. I will help set up a new, high current beamline on the Danfysik ion implanter, which is funded partially through the NSAM-ML Consortium.

MSIPP exposes students to different research projects and provides training to allow the student to grow into a distinguished scientist in science and technology fields related to the National Nuclear Security Administration.

Fellowship Programs

Kelly Moran, Los Alamos National Laboratory (kmoran@lanl.gov) ✦ **Years at LANL:** 2021-Present
Degree: PhD, Statistical Sciences, Duke University ✦ **CSGF:** 2015-2020

The Department of Energy (DOE) Computational Science Graduate Fellowship (CSGF) was much more than a source of funding for me. The CSGF led me to broaden my academic interests, grow my computing capabilities, explore new-to-me groups at Los Alamos National Laboratory (LANL), and accept a scientist job at LANL after finishing my PhD. Perhaps more importantly, the CSGF provided me with the support of everyone involved in the fellowship, including the practicum coordinators, the steering committee, the folks at the Krell Institute managing the fellowship, and my peers.

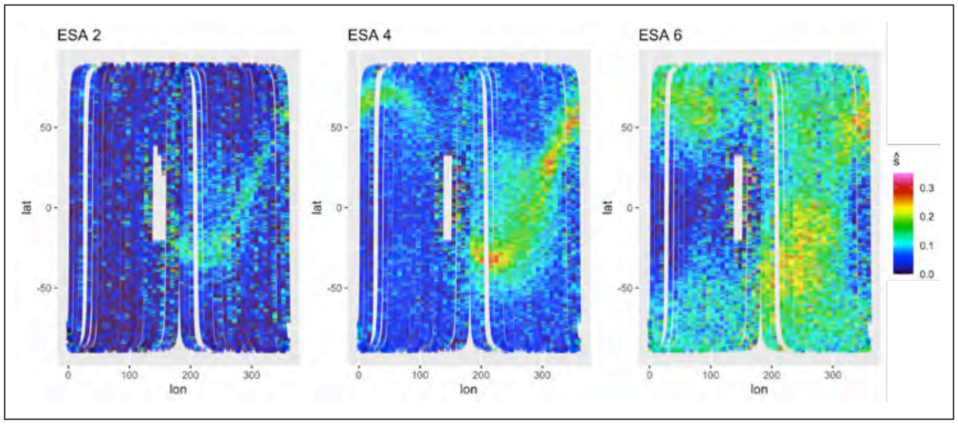


Figure 1. Estimated signal rates for energetic neutral atoms (ENAs) originating from the heliosphere, calculated using data collected by the IBEX-Hi ENA imager at three different electrostatic analyzer (ESA) energy steps. Skymaps generated using these data will be used to discern between competing theories of heliosphere properties, helping us understand why different regions of the heliosphere generate ENAs at different rates.

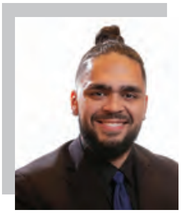
I worked as a post-baccalaureate student at LANL for a year prior to being awarded the CSGF and starting my PhD program at Duke University. At the time, I was a part of the Information Systems & Modeling (A-1) Group and worked on a computational epidemiology team. I fully anticipated that I would research my entire thesis on epidemiology and go back to A-1 after defending. I also wanted to spend as much time as possible in beautiful northern New Mexico working with A-1 while in grad school, enjoying the mesas and mountains (and the Hatch chile). The catch was that the CSGF steering committee, who emphasize breadth, wanted me to do my first practicum with mentors who weren't from A-1.

This breadth requirement meant that I ended up in LANL's Statistical Sciences (CCS-6) Group, working on real-time adaptive acceleration of dynamic experimental science. In short, we were trying to help speed up experiments performed at facilities like SLAC by building statistical emulators for large-scale simulations that could be used in real time. This practicum was my first introduction to Gaussian Processes (GPs), common tools used for statistical emulation. I ended up writing my third thesis chapter about fast approximation methods for Bayesian GP regression. This practicum also was my first introduction to CCS-6. I ended up returning to the group over the next two summers and accepting a scientist job with CCS-6 after finishing my PhD. By pulling me out of my comfort zone and assumed path for a few months, the CSGF helped me to find an even better career fit.

Part of what drew me to the field of statistics is the diversity of problems requiring statistical expertise. In my current role at LANL, I work on cosmology (emulating expensive N-body simulations), heliospheric science (learning about the region between our solar system and greater space), COVID-19 (modeling variant transitions), and underground nuclear explosions (quantifying uncertainty about gaseous breakthrough times). I'm also working to foster a culture of collaboration and warmth within CCS-6 and at LANL. I'm a founder of the Computer, Computational and Statistical Sciences (CCS) Division Early Career/New to LANL group. I also serve as LANL's practicum coordinator, supporting internships for CSGF fellows and encouraging them to consider careers here. I worked with my first summer student this past year and will continue to mentor students moving forward. I'm hopeful that by serving and being visible in these roles, I can help CCS attract and retain more women and LGBT+ folks. Reflecting on my CSGF experience, I'll always be grateful for the networks and opportunities that helped refine my career path in the national laboratories and the personal relationships I formed along the way.

The CSGF led me to broaden my academic interests, grow my computing capabilities, explore new-to-me groups at Los Alamos National Laboratory (LANL), and accept a scientist job at LANL after finishing my PhD. Perhaps more importantly, the CSGF provided me with the support of everyone involved in the fellowship, including the practicum coordinators, the steering committee, the folks at the Krell Institute managing the fellowship, and my peers.

Gabriel Casabona (gcasabona1@gmail.com) ✦ CSGF: 2019-Present
Degree in Progress: PhD, Physics, Northwestern University



Research Topic

Theoretical Astrophysics, Compact Binary Object Mergers

Research Responsibilities

My research responsibilities are theoretical modeling and conducting simulations to test them. These models include a new detonation mechanism for white dwarfs in type Ia supernovae, fully general relativistic fluid model for neutron stars, and the tidal deformation of neutron stars due to gravitational perturbations in binary systems.

Benefits of CSGF

The Computational Science Graduate Fellowship (CSGF) has helped me in a few ways. The first is that it gave me a cushion during a difficult time in graduate school, including switching advisors and medical emergencies. Secondly, the networking opportunities have been fruitful, especially in giving me the opportunity to work at one of the national laboratories along with meeting several leaders in the computational science world and connecting me with like-minded peers.

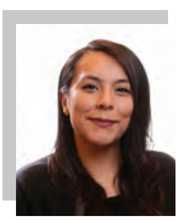
Besides paying our graduate school tuition, with a stipend that rivals most graduate school stipends, the CSGF gives us a support system unique to graduate students. There's an academic allowance to help with costs related to professional development and supplies, something that us fellows agree is highly beneficial and financially advantageous. Connecting us with national laboratories is one of the biggest benefits from the CSGF.

National Laboratory Experience

I completed a practicum at Los Alamos National Laboratory, one of the leading research centers in my field. Outside of my peers in the fellowship, I know very few students who have been as fortunate as I to have the opportunity to conduct research at a major laboratory. The project I worked on is something I've become very excited about, which has led me to learn tons of new physics along with numerical and computational techniques. The people I've met, besides being leading experts in the field, have inspired and mentored me to the point that I now have a much more confident and enthusiastic perspective on my career as a physicist.

The CSGF provides ample networking opportunities, aside from connecting us to our individual laboratory advisers. Our annual meeting in DC gives us the opportunity to listen to and meet with a variety of computational scientists, including alums of the fellowship. They have spoken to us about everything, from how to maneuver our way through careers in laboratory, academia, and industrial settings, to the importance of prioritizing ones mental health to continue being the best scientist, and overall human, possible.

Paulina Rodriguez (pxrodriguez@gwu.edu) ✦ CSGF: 2021-Present
Degree in Progress: PhD, Mechanical and Aerospace Engineering, The George Washington University ✦ Advisor: Dr. Lorena A. Barba



Research Topic

Computational Model Credibility for Medical Device Applications

Research Responsibilities

My research is in the credibility of computational modeling for high-risk applications. I'm developing an example of an end-to-end computational model of a medical device based on risk-informed credibility. An electronic drug delivery system is modeled with computational fluid dynamics and heat transfer. This research doesn't only include model development but also reproducibility, Verification & Validation (V&V), global sensitivity analysis, and Uncertainty Quantification (UQ) using High Performance Computing (HPC). These efforts are part of an ongoing collaboration with the U.S. Food and Drug Administration. Thus, the research goals have a particular focus on credibility and transparency.

Benefits of CSGF

The Computational Science Graduate Fellowship (CSGF) has afforded me the independence to choose a unique research direction while ensuring that I build a strong, well-rounded, computational science foundation. I have access to a community of like-minded, curious, computational science Fellows and professionals who support each other's scientific and personal development. The CSGF Practicum provided me with hands-on research experience at Sandia National Laboratories (SNL). This experience gave me access to a truly collaborative scientific research environment and an applied introduction into HPC. Since my interests are in computational model credibility, the practicum gave me the opportunity to learn from the experts in the most high-risk applications.

What Students Considering CSGF Should Know

The CSGF gives the Fellow the control to find the best research direction that fits their interests. It also provides the support system to succeed in the pursuit of their chosen research direction. From years of experience working with and developing some of the greatest computational scientists, the CSGF has the resources, tools, and motivation to help Fellows develop into strong computational scientists and professionals.

New Contacts, New Opportunities

I conducted my first practicum the Summer of 2022 at SNL. I learned from the experts in V&V, UQ, and credibility processes. I was immersed in the national laboratory collaborative research environment. There I was trained on techniques for developing credibility in high-risk applications that I will translate into high-risk biomedical applications. Although my practicum required COVID-19 safety protocols, I still was able to experience an immersive practicum, where I participated in a truly collaborative research culture where Fellows, mentors, staff, and supervisors were communicating, sharing knowledge, and learning from one another.

Stephanie Miller, NNSA Graduate Fellowship Program (stephanie.miller@nnsa.doe.gov) ✦ **Years at NNSA:** 2022-Present
Degree in Progress: PhD, Plasma Physics, University of Michigan ✦ **LRGF:** 2018-2022

I currently am a member of the National Nuclear Security Administration (NNSA) Graduate Fellowship Program (NGFP). I first learned about the fellowship from a former Stewardship Science Graduate Fellowship (SSGF) and NGFP alumna. She spoke about her career trajectory at one of the SSGF/Laboratory Residency Graduate Fellowship (LRGF) program reviews, and I was inspired to learn more about a future in national security and public policy. Since June, I have been working in Washington, DC at the NNSA headquarters in the Office of Strategic Partnership Programs (NA-10.1). So far, I work to support my office in highlighting and publicizing the innovation that occurs at the national labs as well as interfacing with interagency groups that focus on workforce development and diversity, equity, inclusion, and accessibility (DEIA) initiatives (a huge passion of mine). I still am working to complete my graduate work with hope to defend this winter.

During my residencies at Sandia National Laboratories (Sandia) in Albuquerque, NM, I was able to work on two exciting and impactful projects. For my first residency, I worked on a project to increase laser energy coupling into fusion gas targets for the Magnetized Liner Inertial Fusion (MagLIF) platform. I designed a system to remove a thin plastic window out of the path of a preheating laser. This would allow the energy of the laser to be deposited directly into fuel and not wasted in the process of melting through the window. It also could prevent window material from mixing into the fuel. Increasing this energy coupling can help play a role in increasing the fusion yield for these MagLIF experiments on the Z Machine at Sandia. Figure 1 shows the targets I built to conduct this research as well as some of the key results of achieving and studying this window removal.

For my second residency, I worked to study the wall movement of these MagLIF targets at the OMEGA Laser facility. It was an incredible experience to learn more about the OMEGA laser facilities, interact with the scientists who work there, and have the opportunity to travel to the facility in Rochester, NY as one of the Principal Investigators (PIs) for the shot series. My residencies allowed me to do advanced research that would not have been possible without the support of the LRGF. I am additionally grateful for the mentorship of Matt Gomez, a Sandia scientist and SSGF alum. His involvement as my research mentor and fellowship coordinator for Sandia made my LRGF experience much more educational, rewarding, and fun.

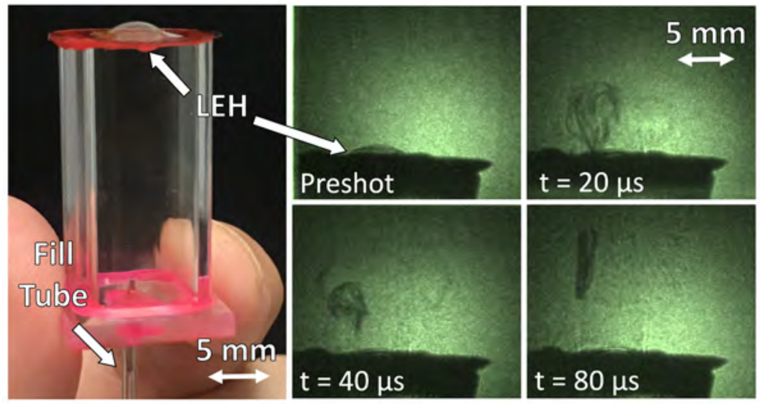


Figure 1. A Laser Gate prototype: When pressurized with target fuel material, the laser entrance hole (LEH) window material domes upward. During laser preheating in a MagLIF experiment (green panel images), the window material weakens, breaks and flaps open away from the preheating laser beam.

My favorite part of the LRGF was the annual program reviews. I enjoyed touring experimental facilities at the national labs. I also found the reviews to be a source of inspiration from other fellows and alumni who are leading the efforts of incredible, cutting-edge research. I learned about my current position during one of the reviews. I urge all current fellows to take advantage of these opportunities to connect with other fellows and alumni who are current and future leaders of our field. The connections I made through the LRGF have not just benefited my career but also have led to friendships I cherish.

I am grateful to the LRGF program and the Krell staff for all their support through the years. The program gave me never-ending opportunities that have drastically molded my career path. I look forward to staying involved in the NNSA, advertising and promoting the LRGF, and attending the annual programs reviews in my newly attained alumna status.

My residencies allowed me to do advanced research that would not have been possible without the support of the LRGF. I am additionally grateful for the mentorship of Matt Gomez, a Sandia scientist and SSGF alum. His involvement as my research mentor and fellowship coordinator for Sandia made my LRGF experience much more educational, rewarding, and fun.

William Brooks (William.C.Brooks@TTU.edu) ✦ LRGF: 2019-Present
Degree in Progress: PhD, Electrical Engineering, Texas Tech University ✦ Advisor: Dr. Andreas Neuber

Research Topic

Vacuum Surface Flashover

Research Responsibilities

Understanding how to prevent electrical arcing within pulsed power systems presents a significant avenue for improving performance of existing systems and a substantial avenue for cost reduction in next-generation facilities. Electrical arcs through a material occur at high thresholds. However, electrical arcs across the surface occur much earlier. Typically, only the final portion of large facilities are kept under vacuum. The transition from the external environment to the vacuum section is one surface particularly vulnerable to breakdown. It is required to be physically larger than surrounding elements to accommodate its electrical weakness. This creates additional burdens and drives larger requirements.

We are developing a test bed that allows multiple simultaneous measurements of breakdown. This encompasses two key challenges: 1) designing a system that is robust enough to push existing, highly optimized geometries to failure, and 2) localizing the event. This enables us to repeatably make electrical and optical measurements of the event. Addressing part 1 is analogous to making the base of a pyramid wider than the tip. Part 2 has not been discussed in literature for the three-dimensional geometry of interest.

My contributions to this project include designing the current geometry of our device under testing, and I have been designing our 2nd generation setup. We are looking to much higher voltages and exploration of scaling laws. We will have improved diagnostic capabilities. My primary research interests lie in making gas density measurements of the onset. This will require fast, non-invasive measurements made by a laser beam and will provide some strong evidence for determining the validity of competing theories of surface flashover.

Benefits of LRGF

I would encourage students to participate in the fellowship programs. The Laboratory Residency Graduate Fellowship (LRGF) is responsible for allowing me to focus on my research without having to divert significant portions of my attention to other occupations. The program has supported some of my equipment and resource costs and has both allowed and encouraged me to engage with the national laboratories and my greater research community.

Kevin Kwock (kevin.kwock@columbia.edu) ✦ LRGF: 2020-Present
Degree in Progress: PhD, Electrical Engineering, Materials Science/Spectroscopy, Columbia University ✦ Advisor: Dr. P. James Schuck

Research Topic

Magneto-optical, Ultrafast, and Near-field Spectroscopy of Low-dimensional Materials

Research Responsibilities

My primary project responsibilities involve studying lanthanide-doped upconverting nanoparticles (UCNPs) for their optical sensing capabilities. UCNPs recently emerged as exciting nanomaterial platforms for all-optical sensing of temperature, pressure, environment, and potentially more. At Columbia, I investigate how UCNPs can have relevant optical sensing functions in imaging nanoscopic surfaces. We employ near-field microscopy techniques that are enabled by conventional scanning probe tools, like the atomic force microscope. By conjugating these tips with a single UCNP to resonantly transfer energy to other nanomaterials during imaging, we can visualize nanoscale topography and nano-optical spectra that would otherwise be inaccessible with a regular optical microscope.

During my Laboratory Residency Graduate Fellowship (LRGF) residencies at the Center for Integrated Nanotechnologies (CINT) and the Laboratory for Ultrafast Materials and Optical Science (LUMOS), I expand on my projects at Columbia by studying other avenues of optical sensing, such as luminescence changes in the presence of strong magnetic fields (up to 7T) and/or when under intense THz irradiation. At CINT/LUMOS, I also employ a plethora of tools ranging from cleanroom fabrication to free-space optics to complete my projects during the residencies.

Benefits of LRGF

I have benefitted enormously from the LRGF program. The overflowing support I receive from the program administrators and the academic flexibility the fellowship has given me has made my tenure extremely positive, freeing up my time at school to pursue other riskier project ideas that are normally not feasible. Secondly, the scientific exposure I have received by being a student at CINT/LUMOS has been an experience unlike any other. Not many doctoral students have the opportunity to simultaneously design their projects and carry them out for extended time periods at a world-renowned, national user facility. The collaborators, mentors, and resources available during this fellowship have been top-notch, and I do not think my doctoral studies could have gone any better.

New Contacts, New Opportunities

Since my undergraduate studies, I spent a total of six summers at Los Alamos National Laboratory and Sandia National Laboratories' CINT through a combination of internships/Graduate Research Assistantships sponsored by MPA-CINT, the Science Undergraduate Laboratory Internship program, and LRGF residencies. One benefit of working at the national laboratories is the experience of being constantly surrounded by a network of scientists I can interact with regularly to solve challenges that come up in my research. Especially during my LRGF residencies, CINT fosters a collaborative and supportive environment which has greatly impacted my research projects as an LRGF fellow.

Alison Saunders, Lawrence Livermore National Laboratory (saunders15@llnl.gov) ✦ **Years at LLNL:** 2018-Present
Degree: PhD, Physics, University of California, Berkeley ✦ **SSGF:** 2015-2018

High energy density physics is characterized by extreme temperatures, densities, and pressures. In my current role as an experimental physicist at Lawrence Livermore National Laboratory (LLNL), I get to add a fourth extreme to the mix: namely, extreme velocities. These are velocities in excess of several kilometers per second (or over several thousand miles per hour) and are so fast that when objects moving at these speeds undergo collisions, the collisions impart enough energy to generate high energy density conditions.

More specifically, I study the high-speed, collisional behavior of ejecta microjets in experiments performed at high power laser facilities, such as the OMEGA Extended Performance laser at the Laboratory for Laser Energetics in Rochester, New York. Ejecta microjets are micron-scale jets of material comprised of particles that travel at extreme velocities. Our experiments use lasers to generate these fast-moving jets from shocked tin samples and then take X-ray radiographs of the interacting jets at different times to create movies of the interactions. Similar to how X-ray images from a doctor's office show contrast on the film between the higher-density bone and lower-density skin, X-ray radiographs of interacting microjets allow us to extract density information to understand collisional behavior as a function of time.

Figure 1 shows X-ray radiographs of two counter-propagating tin ejecta microjets taken at different times before (top image) and after (bottom image) interaction. As seen in the bottom image, collisions between particles comprising the jets generate a large cloud of material around the center region of interaction. This observation contrasts with interactions from jets generated by lower laser drive energies in which lower-density microjets pass through each other without generating such a cloud. The results of this experiment, published in Physical Review Letters,[1] were the first such observations of differences in microjet collisional behavior as a function of shock pressure. My group and I continue to study microjet interactions in the hopes of improving our modeling capabilities of extreme-velocity, small-scale particle collisions.

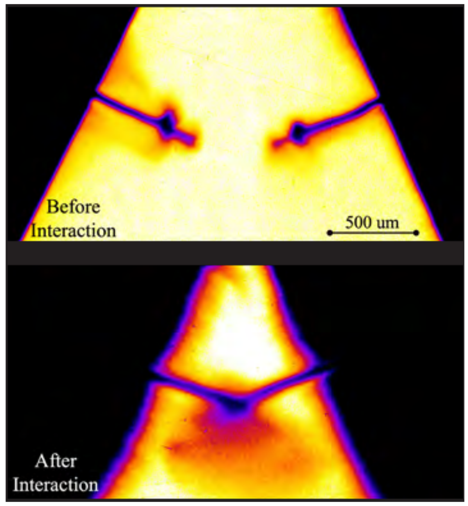


Figure 1. X-ray radiographs of tin ejecta microjets (top) before and (bottom) after interaction. The microjets are moving at speeds in excess of several thousands of miles an hour before colliding and generating a cloud of material.

These microjet collision experiments are the most recent of many high-power laser experiments that I have gotten to be a part of since being awarded with my Stewardship Science Graduate Fellowship in 2015. As a graduate student at in the physics department at UC Berkeley, the fellowship allowed me to perform much of my thesis research in collaboration with scientists at LLNL, and I was immediately attracted by the mission-driven and collaborative nature of these large-scale laboratory experiments. In addition, my practicum at LLNL in 2017 gave me the opportunity to work with a design physicist to learn about how simulations support our understanding of experimental design and data interpretation.

Because of my excitement with the field, I joined LLNL officially as a postdoctoral researcher in 2018 after graduating with my PhD. I now am a staff scientist working both on experiments and simulations of laser-driven, shocked materials. Looking back, my time with SSGF was pivotal in my career trajectory. The fellowship helped me gain valuable skills and, even more importantly, introduced me to many mentors across the NNSA laboratory complex. I believe these fellowships continue to play an important role in attracting top researchers to our field to work in support of our national security missions, and, after my positive experience, I continue to encourage motivated students to apply.

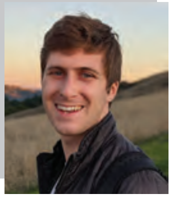
Looking back, my time with SSGF was pivotal in my career trajectory. The fellowship helped me gain valuable skills and, even more importantly, introduced me to many mentors across the NNSA laboratory complex. I believe these fellowships continue to play an important role in attracting top researchers to our field to work in support of our national security missions, and, after my positive experience, I continue to encourage motivated students to apply.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and funded by Laboratory Directed Research and Development 18-ERD-060.

Reference

[1]A.M. Saunders et al., Phys. Rev. Lett. 127, 155002 (2021).

Griffin Glenn (gdglenn@slac.stanford.edu) ✦ SSGF: 2020-Present
Degree in Progress: PhD, Applied Physics, Stanford University ✦ Advisor: Prof. Siegfried Glenzer



Research Topic

High Repetition Rate Laser-driven Ion Acceleration

Research Responsibilities

My research, conducted in the High Energy Density Science Division at SLAC National Accelerator Laboratory, focuses on developing high repetition rate, laser-driven ion beam sources. These beams are produced in the interaction of a high-power laser with a thin, near-solid density target and have many very attractive properties making them suitable for application to important problems in medicine, materials science, and radiography. However, low repetition rates have historically limited the readiness of laser-driven ion beams for these applications. To solve this problem, we are developing continuously refreshed liquid targets that can produce ion beams at up to kHz repetition rates. My day-to-day includes not only technical responsibilities such as design and development of the liquid jet hardware but also conducting and analyzing experiments with these targets at high-power laser facilities nationwide.

Benefits of SSGF

As part of my Stewardship Science Graduate Fellowship (SSGF) practicum at Sandia National Laboratories (Sandia), I had the opportunity to use a brand-new diagnostic instrument called the Ultrafast Pixel Array Camera to perform spatiotemporal characterization of laser pulses on the nanosecond timescale. This was a departure from my thesis research, but it allowed me to broaden my research experience and establish a collaboration with a DOE/NNSA laboratory. In fact, I now am interested in using this instrument to perform additional measurements more closely related to my primary thesis research.

My practicum helped me meet colleagues at Sandia I would never have encountered otherwise, illustrating the value of the practicum in building community. During the annual SSGF/Laboratory Residency Graduate Fellowship Program Review, I made friends and professional connections across disciplines and fellowship years. It was also exciting to meet program alumni and begin to connect with the long-term professional network available through the SSGF program.

What Students Considering SSGF Should Know

The prospect of taking time off from dissertation research for your practicum might initially be worrisome, but the practicum actually is a remarkable opportunity. It’s not common to get a chance to completely step away from your work and return with fresh eyes, so make the most of it! During the practicum you can take a mental break from your dissertation research to cultivate a fresh perspective. You’ll find that the practicum research can be a source of new collaborations or ideas that would not have appeared before.

Sandra Stangebye (sstangebye3@gatech.edu) ✦ SSGF: 2020-Present
Degree in Progress: PhD, Material Science and Engineering, Georgia Institute of Technology ✦ Advisor: Dr. Joshua Kacher and Dr. Olivier Pierron

Research Topic

Investigating Deformation Mechanisms of Metal Thin Films

Research Responsibilities

My research is focused on characterizing the deformation mechanisms of metal thin films using a nanomechanical *in situ* transmission electron microscopy (TEM) testing technique. Since these metal thin films only are 100 nanometer in thickness (1,000 times thinner than the average diameter of a human hair), they exhibit unique properties compared to their bulk counterparts. Understanding the mechanisms during deformation is crucial in order to optimize their mechanical properties. I perform mechanical tests inside the TEM (e.g., *in situ*) to characterize the material microstructure in detail and to capture in real-time the interactions between defects such as dislocations and grain boundaries. These experiments are conducted using a custom-designed microelectromechanical (MEMS) device that utilizes capacitive sensing to measure stress and strain of the specimen. Recently, we have expanded this study to involve irradiated metal thin films to investigate how radiation-induced defects interact with the microstructure to control the macroscale mechanical properties.

Benefits of SSGF

I am very fortunate to be a part of the Stewardship Science Graduate Fellowship (SSGF) community, as it has had an incredibly positive impact on my graduate study experience. Not only has it allowed me to focus on my research without worrying about funding, it has provided the invaluable experience of expanding my skillsets to study different material systems during the research practicum. The practicum also provided an opportunity to expand my PhD thesis project to include investigating radiation-induced property changes in metal thin films. This ended up being quite fruitful for my project which would not have been as easily achieved without the fellowship. I am incredibly thankful to be connected with the community of past and current fellows. I look forward to the lifelong friendships and collaborations that were born out of this fellowship.

What Students Considering SSGF Should Know

To any student considering the SSGF, I could not recommend it more. Even if you do not know if the national laboratory route is the perfect fit for you, I encourage you still to apply. It allows for the opportunity to explore the national laboratory environment before committing to a full-time position. This fellowship is a unique opportunity that very few graduate students benefit from, and it will only enhance your graduate studies.

Fellows

As far as networking goes, my favorite part of having this fellowship is meeting all the amazing fellows. Within my cohort, we have become our own support system of friends. Since graduate life brings with it unique hardships, not to mention what's been happening around the world the past couple of years, having like-minded people in my corner has been nothing short of a blessing. Finally, the administrative staff at Krell takes care of us in ways that rival any fellowship and are truly the best!

Gabriel Casabona, Northwestern University
Computational Science Graduate Fellowship

There are a plethora of subjects important to stockpile stewardship. This multidisciplinary topic requires not only exceptional professionals but cooperation. My residencies have given me the delightful experience of contributing to such an environment. The program has made lasting connections with many existing and future experts.

William Brooks, Texas Tech University
Laboratory Science Graduate Fellowship

I was able to see the collaborative work environment of the national labs and how they tackle very large problems in the national interest. While doing so, I was able to learn and add new tools to my own scientific toolbelt. Each summer I learned new skills that I have incorporated into my own PhD thesis work. Overall, my experiences at the national labs has made me a better scientist and have stimulated my interest to continue working in the dynamic national lab environment.

Griffin Glenn, Stanford University
Stewardship Science Graduate Fellowship

User Facilities

High Pressure Collaborative Access Team—Synchrotron-Based, Experimental Facility for Studying Matter at Extreme Pressure-Temperature Conditions ✦ Advanced Photon Source, Argonne National Laboratory

Authors: Dr. Nenad Velisavljevic (HPCAT-Director@anl.gov) and Maddury Somayazulu (zulu@anl.gov)

It is an exciting time at the High-Pressure Collaborative Access Team (HPCAT) facility. HPCAT was established in the early 2000s with core funding from the National Nuclear Security Administration (NNSA) and, after 22 years of continuous operations, HPCAT is preparing for a significant facility upgrade starting in April of 2023. HPCAT is a synchrotron-based, high-pressure research facility (Figure 1) dedicated to providing cutting-edge, experimental capabilities that enable NNSA laboratories (i.e., Los Alamos National Laboratory, Lawrence Livermore National Laboratory, and Sandia National Laboratories (SNL)), NNSA Academic Programs, and the broader scientific community to investigate matter at pressure-temperature (P-T) extremes using high energy X-rays. In addition to supporting a diverse user community, HPCAT is focused on research and development of synchrotron X-ray techniques for 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 the next generation workforce at the national laboratories. HPCAT currently consists of four simultaneously operational experimental stations (also referred to as beamlines) (Figure 1). The four beamlines have been developed to provide a comprehensive array of experimental platforms for obtaining critical and fundamental experimental data in support of stewardship science and advancing high pressure scientific fields.

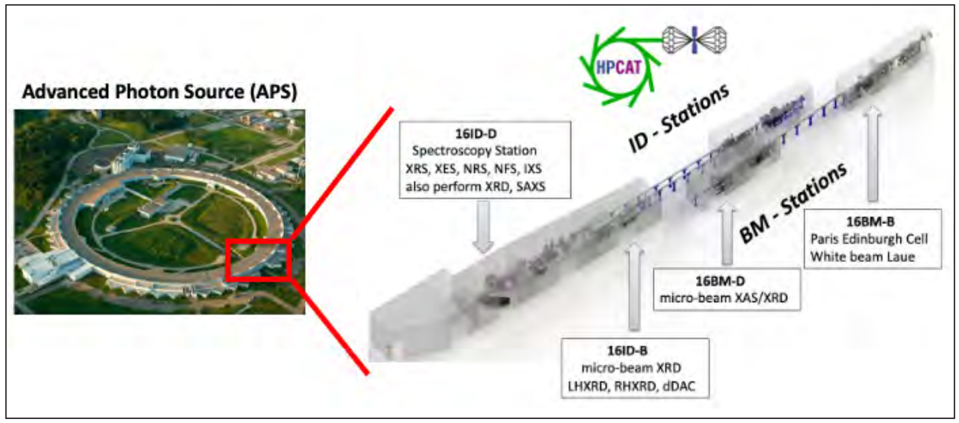


Figure 1. Shown on the left is the synchrotron X-ray Advanced Photon Source (APS), located at Argonne National Laboratory. APS hosts various dedicated experimental facilities, know as Collaborative Access Team (CAT) or sectors. On the right is a close-up view of the HPCAT facility, which is located at sector 16 and consists of numerous experimental stations (labeled as 16ID-D, 16ID-B, 16BM-D and 16BM-B). Each experimental station provides unique X-ray capabilities for studying materials at high pressure conditions. Additional details regarding HPCAT capabilities can be found at https://hpcat.aps.anl.gov/.

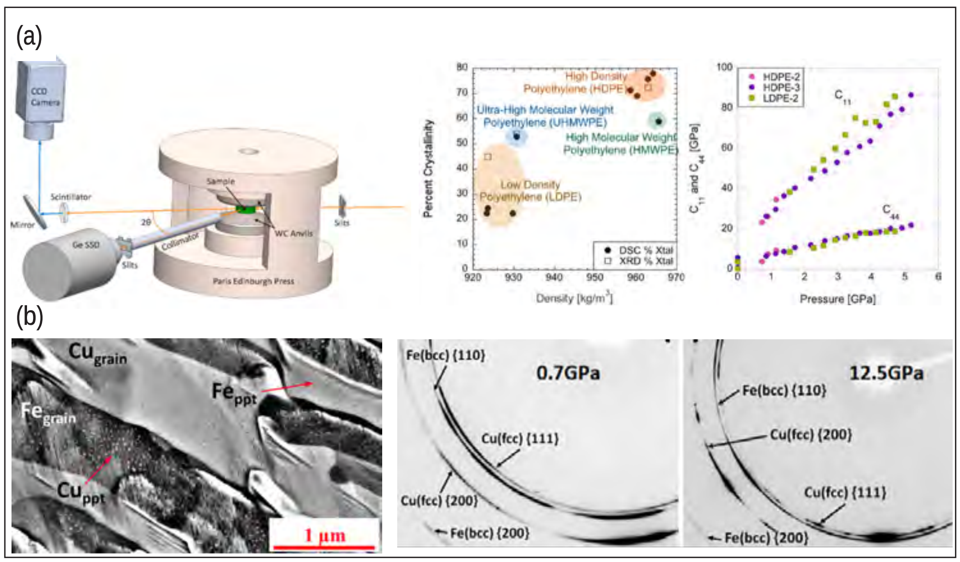


Figure 2.HPCAT platforms are used to support various NNSA laboratory and SSAA experimental efforts. (a) On the left is a schematic of the Paris-Edinburgh press used for in situ pressure dependent measurements, including ultrasound time of flight, X-ray diffraction, and X-ray radiography. On the right are the results of pressure- and temperature-dependent elasticity, described by the tensor Cij(P,T), of polyethylene, measured by the LANL team.[1] (b) On the left is a micrograph showing two phase-separated regions of Cu and Fe (Cugrain and Fegrain) and the presence of precipitates (Cuppt and Feppt) formed during the laser direct-metal deposition (DMD) process. On the right is X-ray diffraction measurement of structural stability and compressibility of Fe and Cu alloy over a broad pressure range.[2]

With over 700 experimental-user visits per year, HPCAT continues to support a robust experimental user program and contributes to vital, NNSA-mission-critical work. Recent measurements by a LANL partner group using the large volume Paris-Edinburg platform at 16BM-B provide accurate characterization of a material's pressure- and temperature-dependent elasticity, described by the tensor, Cij(P,T), for formulating equation of state and strength models (Figure 2(a)). In another effort by the Stewardship Science Academic Alliances (SSAA) Center for Research Excellence on Dynamically Deformed Solids (CREDDS), the team of researchers from CREDDS and HPCAT performed first baseline compression studies of the newly manufactured and unique 50Cu–50Fe alloy. The state-of-the-art, custom-built, direct-metal deposition (DMD)-based additive manufacturing (AM) system at the University of Michigan CREDDS facility was used to manufacture 50Cu–50Fe alloy with tailored properties for use in high strain/deformation environments. Subsequently, the team performed preliminary high-pressure compression experiments to investigate the structural stability and deformation of this material (Figure 2(b)).

In April of 2023, the APS host facility will begin a large-scale upgrade and,

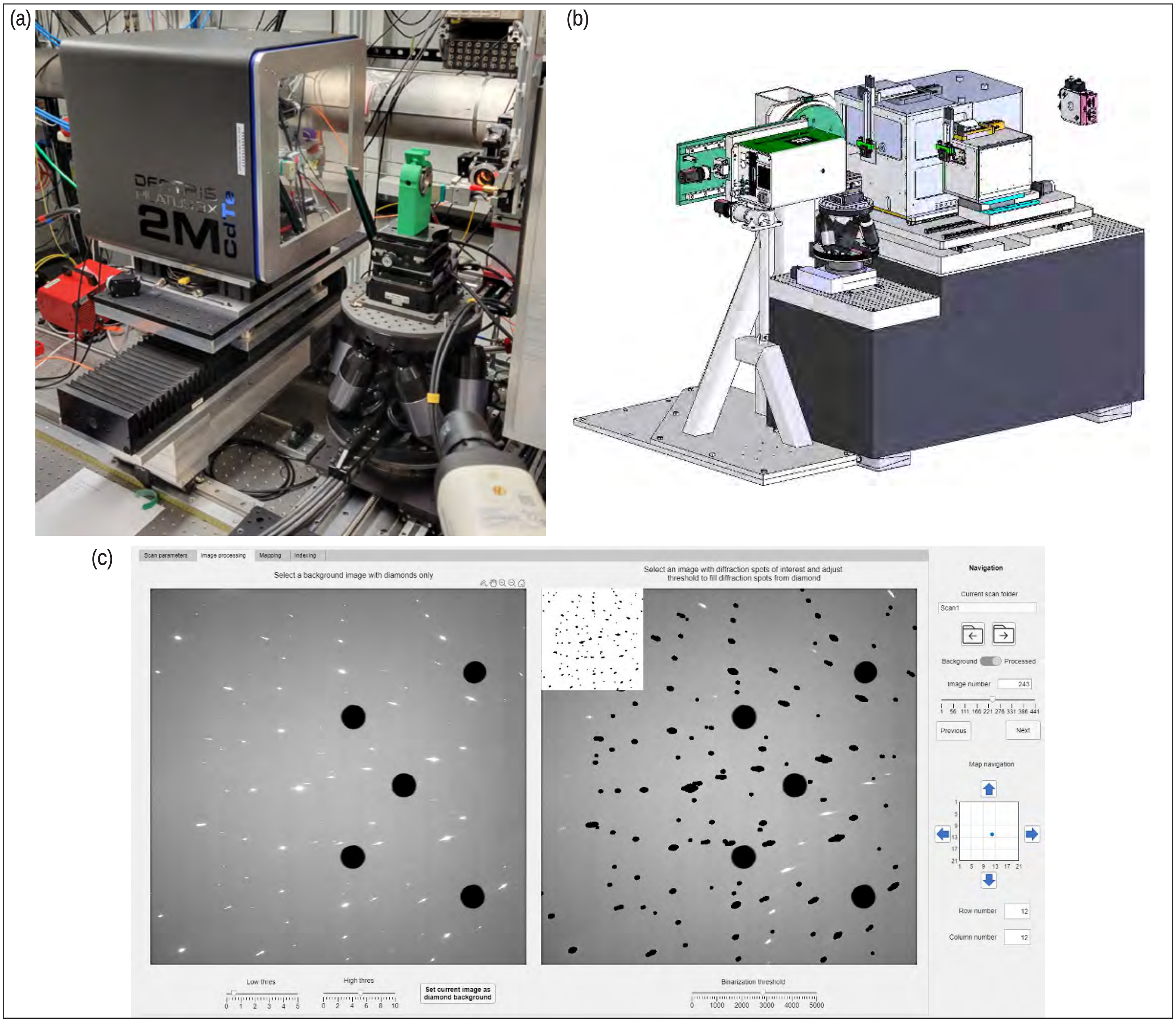


Figure 3. The HPCAT facility is preparing for a major upgrade starting in April of 2023. Various efforts already are ongoing in support of the upgrade: (a) over ~$2M invested in new, state-of-the-art, X-ray detectors, (b) updated and new design of experimental stations/beamlines and (c) development of user-friendly software for optimized data processing.

likewise, HPCAT and all sectors will need to upgrade key infrastructure to ensure compatibility with the new APS upgraded X-ray source. Furthermore, the HPCAT upgrade (HPCAT-U) effort is focused on maintaining competitive leadership in synchrotron-based, high pressure research and continuing to provide cutting-edge experimental platforms in support of NNSA research. Building on top of the $70+M already invested in HPCAT over the last 22 years, HPCAT has been working on an upgrade plan for key infrastructure components and experimental capabilities. With an estimated ~$14M total cost for HPCAT-U, NNSA already has provided $9M toward the upgrade over the last two years and various upgrade efforts are already in progress (Figure 3). HPCAT, along with the APS host facility, is expected to pause user experiments during the upgrade installation efforts with planned user access resuming around April 2024.

References

[1]J. Jordan et al., Polymer 212, 123164 (2021) https://doi.org/10.1016/j.polymer.2020.123164

[2]A. Chatterjee, D. Popov, N. Velisavljevic and Amit Misra, Nanomaterials, 12(9), 1514 (2022) https://doi.org/10.3390/nano12091514

Dynamic Compression Sector: Capability Enhancements Through the 2020s ✦ *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 key needs regarding real-time, multiscale measurements. The DCS uniqueness and extreme versatility arise from the combination of different dynamic compression platforms (plate impact, laser shock, detonation, and special purpose experiments), 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. No existing user facility (worldwide) provides the diversity of experimental capabilities that are available at the DCS.

Figure 1. Single Multilayer Monochromator System in the Laser Shock Station.

Starting in April 2023, the APS will pause operations, and the synchrotron will undergo a major upgrade (APS-U) to produce X-rays having higher brilliance and a much smaller X-ray spot size. Additionally, the separation between X-ray pulses will be reduced from 154 to 77 nanoseconds. After APS-U, the APS will become the first, 4th generation synchrotron light source in the U.S. More X-ray photons will be available at a higher frequency to provide improved insight into time-dependent phenomena and will significantly expand the scientific opportunities for X-ray measurements at the DCS.

To maximize the benefits of the upgraded X-ray beam, the DCS will undertake complementary upgrade activities to address future scientific challenges/needs and to continue as the premier user facility of its kind. Preparations for the APS-U are underway and include capability enhancements and opportunities for the dynamic compression science community to interact with the DCS.

Capability Enhancements

High Energy X-rays: A Single Multilayer Monochromator system (Figure 1) was installed to isolate high energy X-rays (24 and 36 keV) with 1.5% bandwidth and >90% peak efficiency for plate impact and laser shock experiments. During the APS-U, modifications to the X-ray beamline and optics will be made to isolate even higher X-ray energies (>60 keV) to provide users with the ability to investigate higher density and thicker materials – a first-in-class capability for dynamic compression science.

Detector Advancement: The DCS is aggressively supporting innovation and advances in detector technology to ensure the availability of X-ray detectors with at least 13MHz (48-bunch mode) framing capability and high quantum efficiency at 40-60 keV when APS-U comes online.

Driver and Diagnostics Enhancements: Efforts to improve operational efficiency and enhance our current diagnostics and drivers—as well as develop new diagnostics/capabilities—will be undertaken to achieve broader dynamic compression states than are possible currently and improved/novel ways to probe those states in real-time over a large range of length and time scales.

Long-term planning is also underway for future key enhancements, including a 1 kJ laser (with exquisite pulse shaping and excellent reproducibility to permit larger spot sizes and longer pulse durations for dynamic compression of thicker samples) and an office space expansion that will allow users to spend extended time working directly with the DCS staff to explore novel scientific ideas.

Workshop for DCS Users

The DCS will continue its strong emphasis on educating/training new general users to conduct dynamic compression experiments (Figure 2). During the APS-U construction period, workshops for new general users will be scheduled. Users will have the opportunity for conducting experiments at the DCS, although the synchrotron X-rays will not be available, because the DCS dynamic compression capabilities will remain fully functional to undertake dynamic compression studies at the continuum level using the state-of-the-art velocimetry capabilities. In addition, a workshop is planned to define novel scientific opportunities that utilize the enhanced X-ray capabilities of APS-U to ensure that the DCS continues as the premier user facility of its kind (worldwide) through the 2020s.

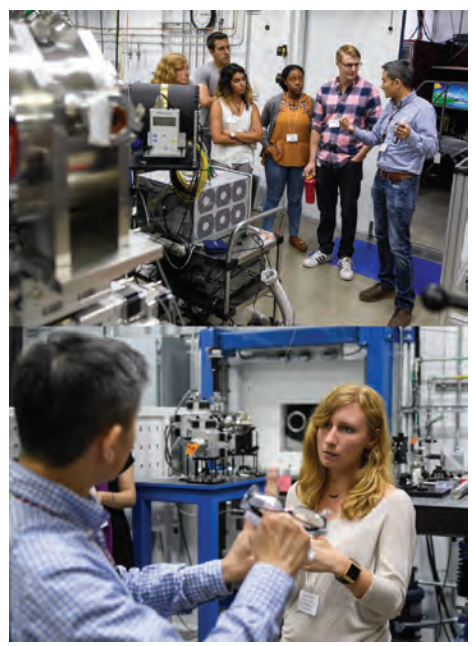


Figure 2. DCS Staff Member, Yuelin Li, conducts a tour of the DCS for workshop participants.

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.

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 (APS) at Argonne National Laboratory, the DCS uniquely integrates state-of-the-art dynamic compression facilities and high energy, synchrotron x-ray capabilities to provide time-resolved, microscopic measurements under high stress impulsive loading. 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). Significant enhancements to the DCS experimental capabilities will be undertaken during the APS-Upgrade. Post APS-U, measurements will be routinely obtained using x-ray energies to 60 keV. For more details visit dcs-aps.wsu.edu or contact Dr. Paulo Rigg (dcs.admin@wsu.edu).

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.

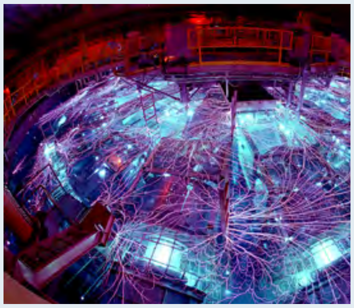
Omega Laser Facility

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 experiments 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.

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.

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.

FY 2023 Funded Grants and Cooperative Agreements

Fellowships

Krell Institute manages the following:
Computational Science Graduate Fellowship
Laboratory Residency Graduate Fellowship
Stewardship Science Graduate Fellowship

High Energy Density Laboratory Plasmas

Colorado State University
Jorge Rocca
Resonant Excitation and Multistage Amplification of Electron Plasma Waves in High Energy Density Plasmas

Cornell University
David Hammer
X-Ray Spectroscopic Studies of Radiative Collapse in X-Pinch Plasmas

Cornell University
Gennady Shvets
Super-Ponderomotive Effects in Ultra-Intense Laser-Plasma Interactions: Towards Novel X-ray and Current Sources

Georgia Tech Research Corporation
Phanish Suryanarayana
Density Functional Theory at Extreme Conditions—Warm Dense Matter from First Principles

Massachusetts Institute of Technology
Johan Frenje
Development of New Advanced X-ray and γ-ray Diagnostics for Inertial-Confinement-Fusion and Discovery-Science Programs at OMEGA and the NIF

Massachusetts Institute of Technology
Chikang Li
Study of Magnetized, High-Energy-Density Hydrodynamics at OMEGA

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

Princeton University
William Fox
Magnetic Reconnection in High-Energy-Density Plasmas

Stanford University
Matthew Edwards
High-Power Photonics Using Adaptively Controlled Plasmas as Diffractive Optical Elements

University of California, Berkeley
Raymond Jeanloz
Tuning Dynamic-Compression Experiments: From Quantum Crystals to Planets

University of California, Los Angeles
Chan Joshi
Generating Ultra-bright VUV and X-ray Sources Beyond Existing Light Sources

University of California, Los Angeles
Warren Mori
Controlling the Nonlinear Optics of Plasmas Using Spatially and Temporally Structured Light

University of California, San Diego
Maria Pia Valdivia Leiva
Development of Talbot-Lau Phase-Contrast X-ray Diagnostics for High Energy Density Laboratory Plasmas

University of California, San Diego
Fabio Conti
Study of Magnetic Field Distribution and Thermal Conduction in Structured, Magnetized Gas Puff Z-pinches

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

University of New Mexico
Mark Gilmore
Exploring the Connection of Magnetohydrodynamic Instabilities to Earlier Electrothermal Instability from Controlled Surface Perturbations on Metal Driven by Intense Current

University of Nevada, Reno
Alla Safronova
Understanding Atomic Properties in HED Plasmas by Studying Line and Continuum Emission from High Z Ions

University of Nevada, Reno
Bruno Bauer
Exploring the Connection of Magnetohydrodynamic Instabilities to Earlier Electrothermal Instability from Controlled Surface Perturbations on Metal Driven by Intense Current

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

University of Nevada, Reno
Roberto Mancini
X-ray Heating, Temperature and Ionization of Photoionized Plasmas

University of Nevada, Reno
Thomas White
Electron-Ion Equilibration in Dense and Quantum Plasmas

University of Rochester
Jessica Shang
Probing Transport Mechanisms in HED Flows

University of Texas at Austin
Todd Ditmire
Investigation of Spherical Radiative Blast Waves in Externally Generated Magnetic Fields

Virginia Polytechnic Institute and State University
Bhuvana Srinivasan
Exploring the Connection of Magnetohydrodynamic Instabilities to Earlier Electrothermal Instability from Controlled Surface Perturbations on Metal Driven by Intense Current

Minority Serving Institutions Partnership Program

American Indian Higher Education Consortium (AIHEC)
American Indian Higher Education Consortium, Lead Recipient
Al Kuslikis

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

Advanced Synergistic Program for Indigenous Research in Engineering (ASPIRE)
Turtle Mountain Community College, Lead Recipient
Austin Allard

Additive Manufacturing Post Processing Partnership (AMP3)
University Of The District Of Columbia, Lead Recipient
Pawan Tyagi

Application of Artificial Intelligence to Cybersecurity for Protecting National Critical Infrastructure (CONCISE)
University Of Texas At San Antonio, Lead Recipient
Guen Chen

Attract, Educate, Train, and Retain Native American and Minority Students in Nuclear & Related Sciences (AETERNAMS)
Nueta Hidatsa Sahnish College, Lead Recipient
Kerry Hartman

Consortium of Advanced Additive Manufacturing Research and Education for Energy Related Systems (CA2REERS)
The University of Texas – Rio Grande Valley, Lead Recipient
Jianzhi (James) Li

Consortium Enabling In- and Ex-Situ-Quality Control of Additive Manufacturing (QCAM)
New Mexico State University, Lead Recipient
Ehsan Dehghan-Niri

Consortium for High Energy Density Science 2.0 (CfHEDS-2)
Florida A&M University, Lead Recipient
Charles Weatherford

Consortium for Laser-Based Analysis of Nuclear and Environmental Materials (LANEM)
Florida A&M University, Lead Recipient
Lewis Johnson

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

Consortium Hybrid Resilient Energy Systems (CHRES)
Universidad Ana G. Méndez-Gurabo, Lead Recipient
Amaury Malavé

Consortium on Nuclear Security Technologies (Connect 2.0)
University Of Texas At San Antonio, Lead Recipient
Elizabeth Sooby

Consortium for Education and Research in Electronics for Extreme Environments (E3C)
University of Texas at El Paso, Lead Recipient
Miguel Velez-Reyes

Enabling Native Researchers and Graduate Engineering (ENRGE)
Navajo Technical University, Lead Recipient
Peter Romine

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

Growing Stems Consortium: Training the Next Generation of Engineers for the DOE/NNSA Workforce (GSC)
Texas Tech University, Lead Recipient
Michelle Pantoya

Integrated Additive Manufacturing – Establishing Minority Pathways: Opportunities for Workforce-Development in Energy Research and Education (IAM-EMPOWEREd)
Florida A&M University, Lead Recipient
Okenwa Okoli

Indigenous Mutual Partnership to Advance Cybersecurity Technology (IMPACT)
Turtle Mountain Community College, Lead Recipient
Chad Davis

Microelectronics & Materials Engineering Education for Nuclear and Cyber Security (MEMENCYS)
University of California, Riverside, Lead Recipient
Shane Cybart

Nuclear Security Science and Technology Consortium (NSSTC)
University of Nevada, Las Vegas, Lead Recipient
Alexander Barzilov

Partnership for Advanced Manufacturing Education and Research (PAMER)
Navajo Technical University, Lead Recipient
Monsuru Ramoni

Partnership for Proactive Cybersecurity Training (PACT)
University Of Arizona, Lead Recipient
Salim Hariri

Partnership for Radiation Studies (PARS)
Alabama A&M University, Lead Recipient
Stephen Babalola

Partnership for Research and Education Consortium in Ceramics and Polymers 2.0 (PRE-CCAP-2)
University Of Texas at El Paso, Lead Recipient
Jack Chessa

The Rio Grande Consortium for Advanced Research on Exascale Simulation (GRANDE CARES)
University Of New Mexico, Lead Recipient
Peter Vorobieff

Scholarly Partnership in Nuclear Security (SPINS)
Alabama A&M University, Lead Recipient
Mebougna Drabo

Successful Training and Effective Pipelines to National Laboratories with Stem Core (STEP2NLs)
North Carolina A&T State University, Lead Recipient
Gregory Monty

Predictive Science Academic Alliance Program III

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

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

Stanford University
Gianluca Iaccarino
Integrated Simulations Using Exascale Multiphysics Ensembles

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

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

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

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

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

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

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

Hydrodynamics, Instabilities, and Hypersonics

Georgia Institute of Technology
Devesh Ranjan
Detailed Measurements of Turbulent Rayleigh-Taylor and Richtmyer-Meshkov Mixing at Extreme Conditions

University of Arizona
Jeffrey Jacobs
An Experimental Study of Rayleigh-Taylor and Richtmyer-Meshkov Instabilities at Large Reynolds Numbers

University of Colorado
Iain Boyd
Computational Modeling of Hypersonic Flow and Material Response in a Free-jet Test Facility

University of Florida, Gainsville
S. Balachandar
Understanding Hydrodynamic Instabilities of Explosively-Driven Multiphase Fronts for Accurate Prediction of Their Complex Structures

University of Michigan
Carolyn Kuranz
Radiation Transport in Strongly Coupled Plasmas

University of Wisconsin, Madison
Riccardo Bonazza
Experimental Investigation of the Richtmyer-Meshkov Instability Coupled with a Chemical Reaction

Low Energy Nuclear Science

Duke University
Alex Crowell
High-precision neutron-induced cross-section measurements on 191,193Ir

Duke University
Sean Finch
Measurements of Precise Fission Cross-section Ratios and Correlations in Fission Observables

Duke University
Calvin Howell
Measurements of Prompt Neutron Differential Multiplicity in Photofission of ^{235}U, ^{238}U and ^{239}Pu

Duke University
Werner Tornow
Measurement and Analysis of Selected Neutron-induced Fission Product Yields for 235U, 238U and 239Pu

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

Michigan State University
Witold Nazarewicz
Microscopic Description of the Fission Process

Ohio University
Carl Brune
Nuclear Reactions and Scattering

Ohio University
Alexander Voinov
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 Rare Isotope Beams for Stewardship Science

San Diego State University
Kenneth Nollett
Scattering and Direct Reactions in a Shell Model Framework

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

University of California, Berkeley
Lee Bernstein
Correlated Neutron-Gamma Data for Stewardship Science

University of Notre Dame
Anna Simon-Robertson
Constraining Neutron-Capture Cross Sections via Direct and Indirect Experimental Methods

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

Properties of Materials under Extreme Conditions and Energetic Environments

Carnegie Institution of Washington
Sally Tracy
Dynamic Compression of Iron Carbide at Exoplanetary Core Conditions

Colorado School of Mines
Amy Clarke
Microstructure Control of Additively Manufactured Metals of Interest to the NNSA Weapons Complex

Harvard University
Stein Jacobsen
From Z to Planets - Phase IV

Harvard University
Isaac Silvera
Metallic Hydrogen: Reflectance, Metastability, and Superconductivity

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

Stanford University
Leora Dresselhaus-Marais
New Operando X-ray Microscope for Movies Resolving the Nanoscale Origins of Defects in Metal Additive Manufacturing

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 California, San Diego
Brian Maple
Novel d- & f- Electron Materials Under Extreme Conditions of Pressure, Temperature, and Magnetic Field

University of Florida
Douglas Spearot
Understanding the role of Elastodynamic Effects on Shock Induced Plasticity via Discrete Dislocation Dynamics Simulations

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

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

University of Rochester
Niaz Abdolrahim
Time-Resolved Classification of X-ray Diffraction Data Using Deep-Learning-Powered Computer Vision Techniques

University of Texas at Austin
Michael Downer
Radiography of High Energy Density Phenomena Using X-rays from Laser Plasma Accelerators

Washington State University
Hergen Eilers
Real-time Monitoring of Chemical Reactions at Subsurface Locations in Optically Opaque and Highly Scattering Samples

Washington State University
Choong-Shik Yoo
Chemistry of Dense Planetary Mixtures at Extreme Conditions

Radiochemistry

Clemson University
Brian Powell
Combined Field and Laboratory Studies of Plutonium Aging and Environmental Transport

Clemson University
Scott Husson
Improving the Sensitivity and Precision for Plutonium Isotope Ratio Measurements by Thermal Ionization Mass Spectrometry Using a Novel Polymer Fiber Platform

Duke University
Jason Amsden
Virtual-Slit Cycloidal Mass Spectrometer for Portable Rapid Ultra-Trace Isotope Ratio Analysis of Actinides

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

University of Notre Dame
Amy Hixon
Actinide Center of Excellence

Washington University in St. Louis
Rita Parai
Seeing Through the Fission Phase 2: Multi-Modal Analysis of Actinides and Noble Gas Isotopes in Geological Samples

User Facilities

Dynamic Compression Sector
Argonne National Laboratory
Yogendra Gupta, WSU

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

Omega Laser Facility
University of Rochester Laboratory for Laser Energetics
Mingsheng Wei

NNSA
National Nuclear Security Administration
DEFENSE PROGRAMS