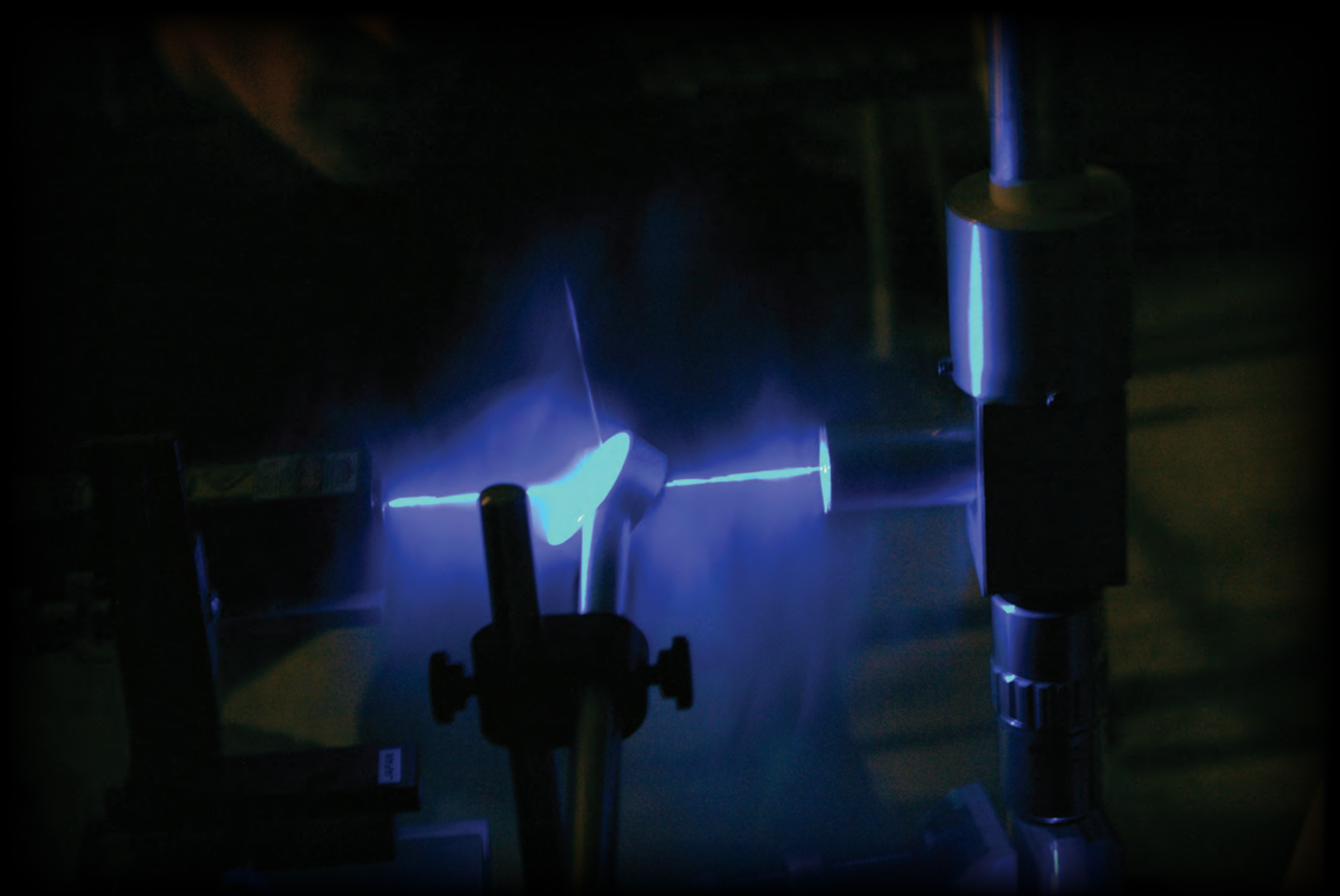
DOE/NA-0069

2018 Stewardship Science Academic Programs Annual

- Stewardship Science Academic Alliances
- High Energy Density Laboratory Plasmas
- National Laser Users' Facility
- Predictive Science Academic Alliance Program II

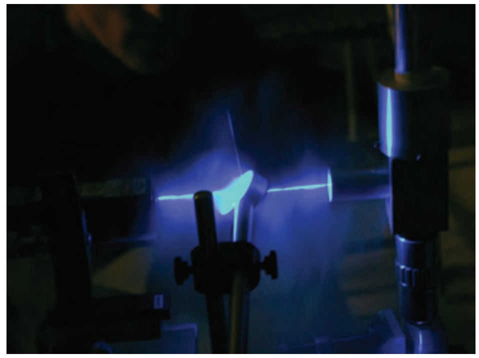


National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY

On the Cover

Transmission and reflectance of a blue-light laser beam (coming from the left) at a dichroic mirror. The laser and optical system is used in determining the static pressure in a diamond anvil cell (DAC) at room temperature. The transmitted beam is redirected downward to the 300-micrometer-sized sample space within a DAC where small chips of ruby are excited by the blue-light laser beam. The excitations in the ruby chip manometers give rise to an emitted red-light fluorescence (not shown) which is picked up by a spectrometer. The peak wavelength of the ruby fluorescence is used to determine the pressure within the sample space of the DAC before and after electrical resistivity measurements are performed in a low-temperature cryostat.



— Image courtesy of Dr. M. Brian Maple, University of California, San Diego

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2018 Stewardship Science Academic Programs Annual

NNSA Office of Research, Development, Test, and Evaluation

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The Stewardship Science Academic Programs Annual is produced by the NNSA Office of Research, Development, Test, and Evaluation. It features select research conducted by the following NNSA-supported research programs: Stewardship Science Academic Alliances, High Energy Density Laboratory Plasmas, National Laser Users' Facility, and the Predictive Science Academic Alliance Program II. For more information, visit www.nnsa.energy.gov/stockpilestewardship.

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Published February 2018

National Nuclear Security Administration

"NNSA developed the Stewardship Science Academic Programs more than a decade ago to support both students and their professors in developing the technical skills required by the SSP; and, to build a pipeline of professionals with key expertise and technical know-how to ensure the integrity of the future nuclear deterrent."

— Dr. Kathleen B. Alexander

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

The primary mission of NNSA is to maintain a safe, secure, and effective nuclear deterrent. Since 1992, we have accomplished this mission without nuclear explosive testing through the expert application of experimental science, engineering, and computational capabilities. This science-based approach underpins the Stockpile Stewardship Program (SSP).

To ensure that this science-based approach remains effective into the future, it is necessary to train individuals in key specialized scientific and engineering disciplines. NNSA developed the Stewardship Science Academic Programs (SSAP) more than a decade ago to support both students and their professors in developing the technical skills required by the SSP; and, to build a pipeline of professionals with key expertise and technical know-how to ensure the integrity of the future nuclear deterrent. The SSAP is essential to building the cadre of experts that will be the future stockpile stewards that will reside at national laboratories, sites, plants, and federal headquarters. We are pleased that many past participants from the SSAP have chosen a career with NNSA, with many choosing service at the national laboratories. These talented scientists and engineers are a vital part of our current and projected future success.

Work conducted in the SSP is exciting and cutting-edge and includes areas such as materials science studies to understand the fundamental properties of key materials and how these materials are affected by pressure and temperature extremes. A subset of this work includes research and experimentation to understand how manufacturing processes can affect the fundamental structure of materials and to understand how advanced manufacturing (including 3D printing) affects the resulting materials properties. Another exciting area is the use of lasers to create plasma conditions in laboratory experiments to understand how engineered systems are affected under these intense, plasma conditions and how various components of the systems interact. Work also is conducted in the design and engineering of one-of-a-kind, state-of-the-art diagnostics that allow data to be collected from these experiments—experiments that occur in extreme pressure and temperature regimes. The design and engineering of those diagnostics has yielded amazing advances and represents an entire field of study unto itself. These are only a few examples of the exciting work that occurs at the NNSA national security laboratories under SSP.

World-class, state-of-the-art theoretical, computational, and experimental science and technology is key to maintaining the effectiveness of our nation's nuclear deterrent. The high quality of work performed under the SSAP is reflected in this 2018 Stewardship Science Academic Programs Annual, and the work illustrates the success of the SSAP in building the pipeline of talent and new ideas so vital to the future security of our Nation. The work presented in this annual, however, represents only a fraction of the outstanding work done in the SSAP. Simply, we cannot fit it all in.

To all of you, I extend my best wishes for continued future successes and congratulations on your successes to date.

Dr. Kathleen B. Alexander

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

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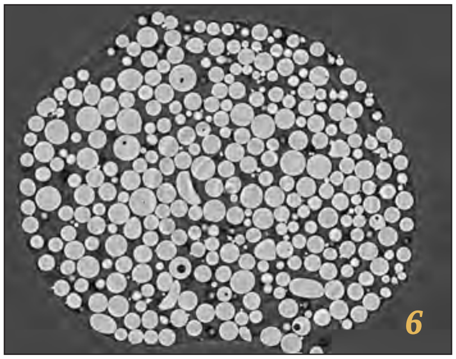

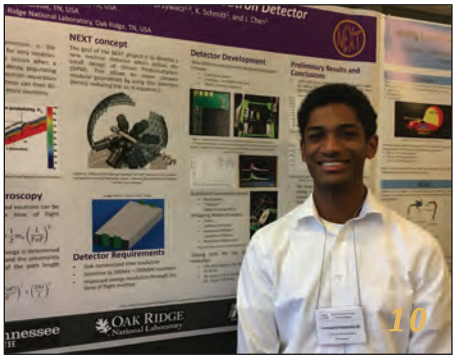

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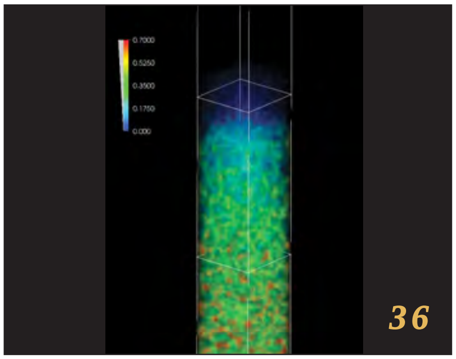

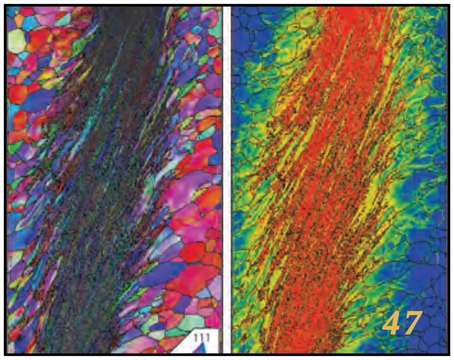

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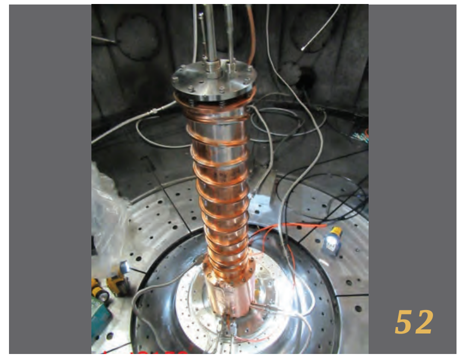

Feature Articles

Grants and Cooperative Agreements

Stewardship Science Academic Programs

— Training the Next Generation

Mitchell Friend, Washington State University graduate student, performs experiments with Tc(IV) under inert atmosphere.

The Nation's nuclear weapons stockpile is a vital part of our national security infrastructure. Ensuring that this deterrent is second to none requires the best science and technology, especially in this post-nuclear-testing era. Having top tier scientists and engineers in the areas critical to stockpile stewardship is the only way to ensure the best science and technology. The National Nuclear Security Administration (NNSA) supports this effort through the Office of Research, Development, Test, and Evaluation's Stewardship Science Academic Programs (SSAP).

In this annual report, some of the outstanding work performed under the SSAP is highlighted. The SSAP includes the following programs:

- Stewardship Science Academic Alliances (SSAA) Program;
- High Energy Density Laboratory Plasmas (HEDLP) Program;
- National Laser Users' Facility (NLUF) Program; and
- Predictive Science Academic Alliance Program II (PSAAP II).

These research elements support U.S. research at universities in scientific areas important to stockpile stewardship. A fundamental objective is the support and training of doctoral and masters degree students studying science and engineering, with a view towards some of these students becoming future stewards of the stockpile. A second fundamental objective is to connect highly skilled academic and NNSA scientists, so that new ideas and techniques can be introduced into the NNSA's arsenal. A third fundamental objective is to ensure that there is a strong community of technical peers throughout the country, external to the NNSA national laboratories, i.e., Lawrence Livermore National Laboratory, Los Alamos National Laboratory, and Sandia National Laboratories, that is capable of providing peer review, scientific competition, and depth and breadth to the basic fields of research important to NNSA.

The SSAP also includes the Stewardship Science Graduate Fellowship (SSGF) Program and the Computational Science Graduate Fellowship (CSGF) Program, the latter jointly sponsored with the U.S. Department of Energy's (DOE's) Office of Science. The SSGF and CSGF programs support PhD students in areas of interest to stockpile stewardship. They provide a yearly stipend, tuition fees, and an academic allowance. This issue highlights an alumnus and four students from the SSGF Program. These individuals share information about their experiences as fellows and how the program has helped shape their careers. For more information about these programs, please visit http://www.krellinst.org/fellowships.

Stewardship Science Academic Alliances (SSAA) Program

Launched in 2002, this program, emphasizes areas of fundamental research and development that are relevant to the Stockpile Stewardship Program mission, typically underfunded by other federal agencies, and for which there is a recruiting need at the NNSA national laboratories. Advanced experimental activities are supported through Centers of Excellence and/or research grants in the fields of properties of materials under extreme conditions and/or hydrodynamics; low energy nuclear science; radiochemistry; and high energy density physics.

The 2017-2018 Stewardship Science Graduate Fellowship Class. Front row, left to right: Emily Abel, Michigan State University and Erin Nissen, University of Illinois at Urbana-Champaign. Back row, left to right, Paul Fanto, Yale University; Gabriel Shipley, University of New Mexico; and Gil Shohet, Stanford University.

High Energy Density Laboratory Plasmas (HEDLP) Program

The NNSA's Office of Inertial Confinement Fusion and the DOE's Office of Fusion Energy Sciences established this joint program in 2008. It involves the study 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). Some of the areas of interest include high energy density hydrodynamics, radiation-dominated hydrodynamics, material properties, nonlinear optics of plasmas, laser-plasma interactions, and warm dense matter.

National Laser Users' Facility (NLUF) Program

The primary purpose of this program is to provide facility time for university- and business-led high energy density experiments on the Omega Laser Facility at the Laboratory for Laser Energetics, University of Rochester. Through this program, two of the world's premier laser systems for high energy density research, OMEGA and OMEGA EP, are accessible to a broad community of academic and industrial research interests, for use as tools for conducting basic research experiments in both low and high energy density physics and laser-matter interactions, and in providing research experience necessary to maintain a cadre of trained scientists to meet the Nation's future needs in these areas of science and technology.

Predictive Science Academic Alliance Program II (PSAAP II)

The primary focus of this program is the emerging field of predictive science, i.e., the application of verified and validated computational simulations to predict the behavior of complex multiscale, multiphysics systems, with quantified uncertainty. This is potentially applicable to a variety of applications, from nuclear weapons effects to efficient manufacturing, global economics, to a basic understanding of the universe. Each of these simulations requires the integration of a diverse set of disciplines; each discipline in its own right is an important component of many applications. Success requires using the most powerful computing systems. Consequently, a key component is computer science research (on both software and algorithmic frameworks) that will contribute to effective utilization of emerging architectures leading to exascale.

NNSA Centers of Excellence

Center of Excellence (sen-ter of ek-suh-luh ns) n. multi-investigator team; multiple academic institutions; addresses an over-arching theme or themes of interest within a topical research area relevant to the Stockpile Stewardship Program; attracts high caliber graduate students and trains them in areas critical to stockpile stewardship; provides students with exposure to researchers and the environment of the NNSA National Laboratories. A Center of Excellence conducts research to address the scientific areas of interest as a team, in a manner that is more efficient and effective than by the members of the team acting separately.

The Department of Energy's National Nuclear Security Administration has named Cornell University and the University of Notre Dame as two of the Stewardship Science Academic Alliances (SSAA) Centers of Excellence program funding recipients for their work in High Energy Density Physics and Radiochemistry.

Cornell University's Multi-University Center of Excellence for Pulsed-Power-Driven High Energy Density Science will be led by Drs. David Hammer and Bruce Kusse. The mission of this Center is to carry out fundamental studies of High Energy Density (HED) plasmas produced by pulsed power generators. The principal objectives of this multi-university research center are to improve the understanding of the properties of dense, high temperature plasmas, especially in the presence of strong magnetic fields, while training the next generation of HED research scientists.

The University of Notre Dame's Actinide Center of Excellence (ACE) will be led by Dr. Peter Burns. The research conducted at ACE will integrate both experimental and computational approaches to analyze radioactive materials, including the elements americium, neptunium, plutonium, and uranium, taking advantage of specialized facilities developed at Notre Dame. Further, the team of researchers will focus on three specific themes: the properties and structure of nanoscale radioactive materials, the thermochemistry, or heat energy, associated with these materials, and how nanoscale nuclear materials react in various chemical environments. They will collaborate with other renowned research institutions, including Northwestern University, Oregon State University, the University of Minnesota, and Washington State University. A major goal of the center is to support workforce development as it pertains to Stockpile Stewardship. Researchers will train graduate students, postdoctoral scientists, and engineers to plan, set up, and conduct safe and efficient experiments with radioactive materials.

Other proposals have been selected for negotiation leading to potential award and will be announced once awarded.

> ***"These cooperative agreements insure a pipeline of the next generation of scientists in areas of relevance to the stockpile stewardship mission."***
>
> *— Dr. Kathleen B. Alexander*
> Assistant Deputy Administrator for Research, Development, Test, and Evaluation

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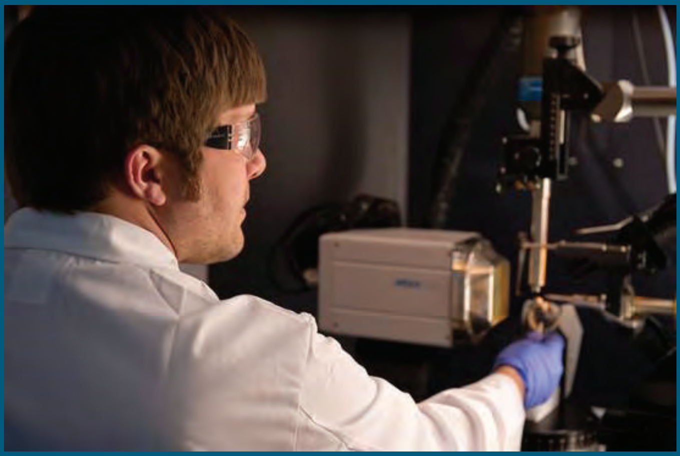
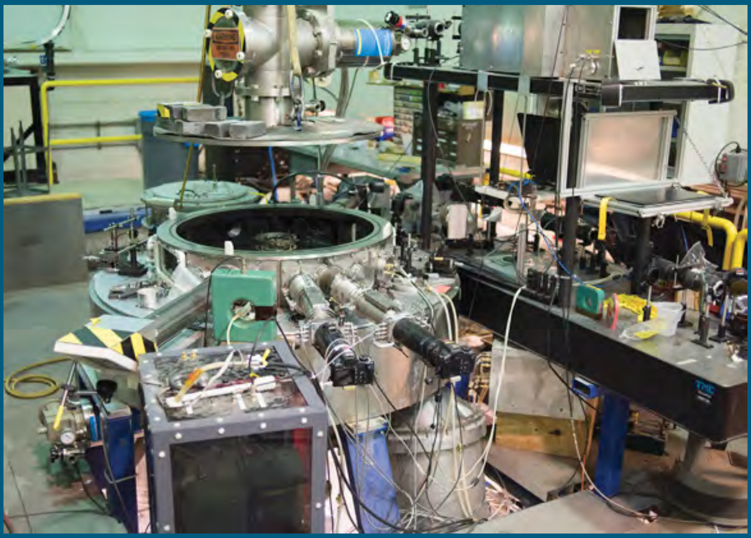


X-ray diffraction is a powerful tool for elucidating the atomic-scale structure of actinide materials. Here, a PhD student prepares to collect data for determining the structure of a compound that contains nanoscale uranium-based clusters.

— University of Notre Dame



*The Cornell Beam Research Accelerator is used in the Laboratory of Plasma **Studies to deliver 150-nanosecond current pulses to various configurations** of metal foils, cylinders, and gas puffs in order to produce high energy density plasmas.*

— Cornell University

Stewardship Science Academic Alliances

Automated Screening of Powders for Additive Manufacturing of Metals

Carnegie Mellon University ◆ PIs: A.D. Rollett (rollett@cmu.edu) and R.M. Suter (suter@cmu.edu) ◆ Author: H. Liu (hel1@cmu.edu)

This SSAP project works towards optimal processing of additive manufactured (AM) metals for high strain rate properties. This is their second year with the program.

The SSAP program allows the principal investigators to expand research on AM metals and to bring new tools to bear to characterize powders used in laser bed AM. With SSAP support, graduate student in the Physics Department He Liu has developed a computational method to screen tomographic images of powder compacts and characterize the degree of porosity present. He has become an expert in the application of machine learning (ML) and has explored the strengths and weaknesses of tomography reconstruction algorithms and post-processing software. These skills will be useful in his future research activities.

Powder bed AM builds three-dimensional (3D) parts by melting metallic powders with either a high power laser or an electron beam. Recent work[1] using synchrotron x-ray computed tomography (CT) has shown that porosity inside powder particles can be transferred to final products, even after post-build treatments, to remove pores, trapped gas can reform voids at high temperatures. Pores are property limiting features for high strain rate applications of interest to NNSA. Thus, quantitative CT characterization can be a critical tool for quality control of AM powders and resulting parts. The goal is to develop automated procedures to identify pores within particles and to statistically characterize the data. This procedure[2] enables screening of large numbers of powders from different processing methods, manufacturers, and production batches. To the best of our knowledge, this is the first time that voids inside particles have been segmented such that pore sizes can be associated with particle sizes.

Thanks to the availability of copious high energy x-rays at the Advanced Photon Source (APS), a 1.5 mm^3 volume of metal powder pack can be measured with 0.65 µm resolution in two minutes. Reconstructions use Tomopy, a python package developed at the Advanced Photon Source, and have a total data size of over 40 Gb. A single slice is shown in Figure 1. To analyze the reconstructed dataset, we need to isolate or segment the powder particles from the background. This turns out to be difficult for two reasons: First, the distribution of density in the particles and in the background can overlap, making segmentation with simple thresholding poor. Second, the large data volume makes it hard to implement other methods, especially if we want to use the complete 3D data set to obtain optimal statistics.

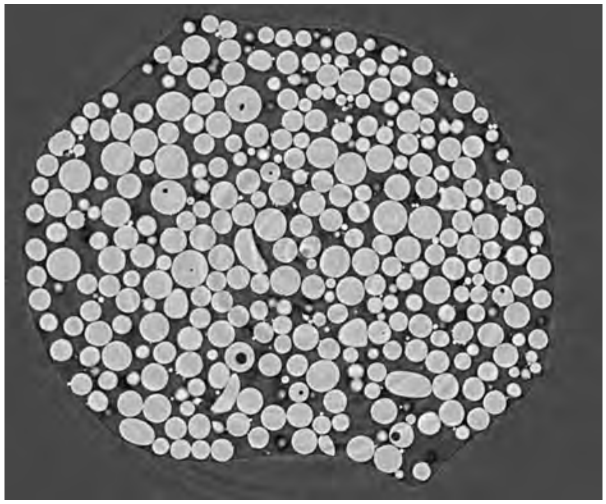


Figure 1. Single slice of a tomographic reconstruction. Gray scale is the reconstructed material density.

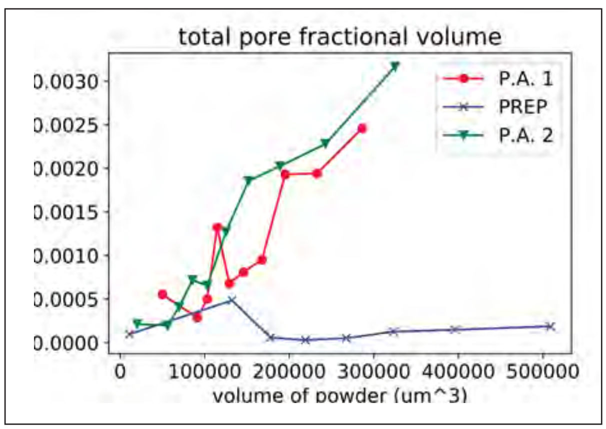


Figure 2. Fractional porosity for three powder compacts. P.A.: plasma atomized, PREP: plasma rotating electrode process powder.

ML allows algorithms to learn from example features and complete complex tasks in an automated way. ML-based segmentation can classify each reconstructed voxel based not only on its density but also on the surrounding environment. The algorithm applies a variety of filters and is trained through manually specified examples to distinguish particles from background. In this way, a binary output of segmented 3D images can be obtained. Pores are seen as background but can be identified as regions that are surrounded by high density voxels in all directions. For statistical analysis, these binary datasets are well handled by the commercial software Avizo.

Figure 2 shows, for three different powder samples, the average fraction of the volume inside powder particles that is occupied by porosity as a function of particle volume. For the plasma atomized powder, larger powder particles tend to have a larger fraction of pore volume. However, the plasma rotating electrode process appears to avoid this trend and leads to much lower porosity independent of particle size. Additional datasets are currently being processed and additional processing approaches are being investigated.

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[2] H. Liu, R. Cunningham, A.D. Rollett and R.M. Suter, "Tomographic Screening of Powder Compacts for Pore Characterization," in preparation.

Spectroscopic and Nuclear Magnetic Resonance Studies of Screening in Compressed Rare Earths and Rare Earth Compounds

University of California, Davis ◆ PIs: Nicholas Curro, Warren Pickett, and Richard Scalettar (scalettar@physics.ucdavis.edu)

The field of magnetic materials is amongst the most rapidly evolving areas of condensed matter physics and has tremendous technological relevance. The objective of this project is an investigation of several classes of magnetic materials—rare earths and their compounds, heavy fermions, and iron-pnictide superconductors—which exhibit many unusual and potentially important properties. The application of high pressure constitutes one of the most important external parameters which can tune these systems through different electronic, magnetic, and superconducting phases. At the same time, spectroscopy and nuclear magnetic resonance (NMR)—a process in which nuclei in a magnetic field absorb and re-emit electromagnetic radiation—performed at high magnetic field and to ultra-low temperatures are able to track the changes induced as the atoms are squeezed closer. A key element of our work is a close collaboration with scientists at Lawrence Livermore National Laboratory and the National High Magnetic Field Laboratory. Six current students are involved with the project. Four former students hold positions at the NNSA national laboratories. "Support from the SSAP has brought the PIs, and their students, into collaborations with outstanding colleagues at NNSA labs, greatly enhancing our research and education missions," said Richard Scalettar, Professor of Physics.

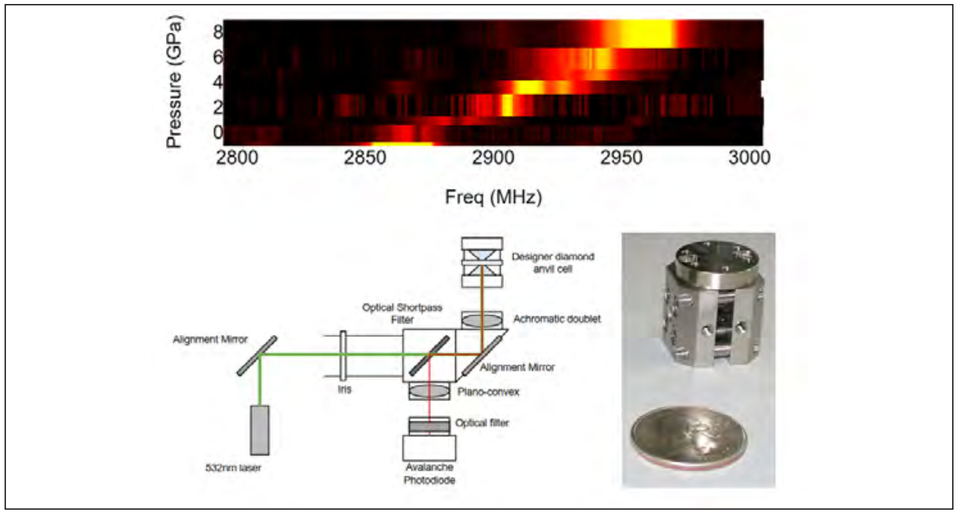

Figure 1. Top: Optically-detected magnetic resonance spectrum versus pressure in the diamond anvil cell (DAC). Bottom: Sketch of the experimental setup and the DAC itself.

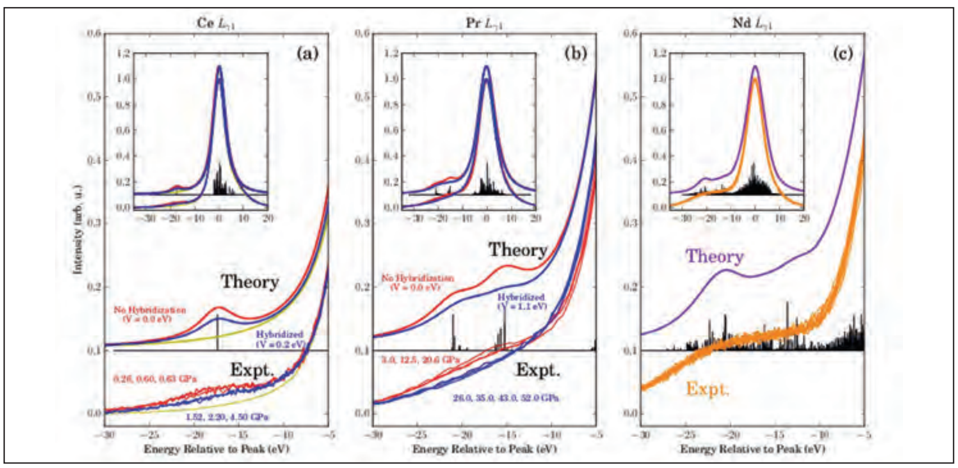

Figure 2. The satellite region of the experimental and calculated x-ray emission spectra for light lanthanide metals. The red (blue) curves are at low (high) pressure. Insets show the full $L\gamma_1$ spectra.(a) The yellow curves are results of lanthanum (no f electrons). (c) The Nd $L\gamma_1$ spectra do not change with pressure up to 43 GPa. Here, experimental and theoretical results are shown as orange and purple respectively. The calculated spectra are shifted by +0.1.

Magnetic Resonance of Nitrogen Vacancies

Optically detected magnetic resonance of nitrogen vacancy centers in diamond offers novel routes to both DC and AC magnetometry in diamond anvil cells under high pressures (>3 GPa). However, a serious challenge to realizing experiments has been the insertion of microwave radiation into the sample space without screening by the gasket material. We utilize designer anvils with lithographically-deposited metallic microchannels on the diamond culet as a microwave antenna. We detect the spin resonance of an ensemble of microdiamonds under pressure, and measure the pressure dependence of the zero field splitting parameters. These experiments enable the possibility for all-optical magnetic resonance experiments on sub-μL sample volumes at high pressures.

X-ray Spectroscopy of Light Lanthanide Metals

The chemistry of lanthanides is of critical importance to fields from catalysis, to high-temperature superconductivity and bioscience. Despite a rich history, theoretical treatment remains a fundamental challenge. The difficulty stems primarily from the underlying nature of *f*-electron states. Using the satellite structure of the $L\gamma_1$ line in non-resonant x-ray emission spectra, we probed the high-pressure evolution of the bare 4*f* signature of the early light lanthanides at ambient temperature. For Ce and Pr, the satellite peak experiences a sudden reduction concurrent with their respective volume collapse transitions. These results are supported by calculations using state-of-the-art extended atomic structure codes.

References

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Novel *d*- and *f*-Electron Materials Under Extreme Conditions of Pressure, Temperature, and Magnetic Field

University of California, San Diego ◆ PI: Professor M. Brian Maple (mbmaple@ucsd.edu)

The objectives of this SSAA project are to investigate the behavior of matter under extreme conditions of pressure, temperature, and magnetic field, obtain a greater understanding of the physics of transition metal, lanthanide, and actinide based *d*- and *f*-electron materials, and train the next generation of scientists in static high-pressure experimental techniques in support of stockpile stewardship. During the past year, one postdoctoral researcher, two graduate students, and one undergraduate student have been supported by the SSAA grant. Since the beginning of this project in 2003, three former group members have held postdoctoral appointments and three are currently staff members at Los Alamos National Laboratory or Lawrence Livermore National Laboratory. Studies of the properties of novel *d*- and *f*-electron materials under conditions of high pressure, high field, and low temperature provide important information that will contribute to the understanding of unconventional superconductivity, magnetism, and other correlated electron phenomena. Twenty-five students and postdocs in this program have gained experience in methods of materials synthesis and high-pressure techniques using piston-cylinder, Bridgman anvil, and diamond anvil cells for performing transport and magnetic measurements at pressures up to ~100 GPa.

During the past year, experiments were performed at high pressures and in high magnetic fields on novel materials that undergo transitions into several types of ordered states at low temperatures. Perhaps the most striking of these ordered states is "superconductivity" (SC), a phenomenon in which mobile electrons in certain metals form electron pairs (so-called "Cooper pairs") that condense into a macroscopic quantum state below the superconducting critical temperature T_c, in which the electrical resistance of the metal vanishes, i.e., the metal becomes a perfect conductor of an electric current. Another type of order is magnetic order, where magnetic moments (tiny "bar magnets") on atoms with partially-filled *d*- or *f*-electron shells spontaneously align in certain configurations when cooled below the magnetic ordering temperature T_M. A familiar example is "ferromagnetism," where the magnetic moments align in the same direction; this occurs in iron and is responsible for its magnetic field. Another example is "antiferromagnetism" (AFM) in which the magnetic moments on neighboring atoms align in opposite directions. A particularly interesting example is "hidden order" (HO), an unknown type of order found in the *f*-electron compound URu_2Si_2 below $T_o = 17.5$ K.[1,2] While many types of measurements (e.g., electrical, thermal, magnetic, and spectroscopic) have been performed on URu_2Si_2, and numerous theoretical models have been proposed to describe the nature of the HO phase,[2] the identity of the mysterious HO phase has eluded researchers for more than three decades![2] As this compound is further cooled below $T_c = 1.5$ K, an unconventional type of SC emerges within the HO phase.[1,2]

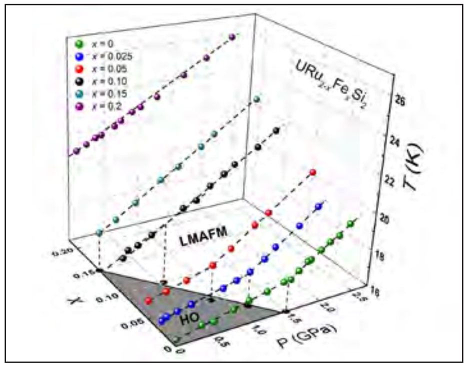

Figure 1. T vs. x phase diagram for single crystals of $URu_{2-x}Fe_xSi_2$.[5]

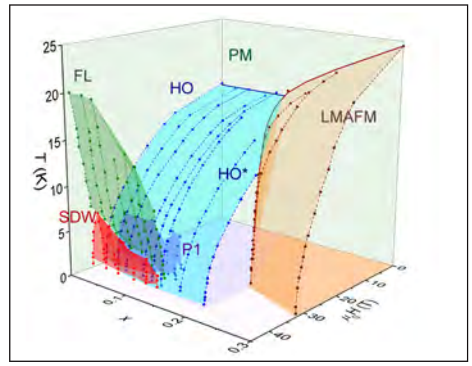

Figure 2. 3D T–x–H phase diagram for single crystals of $URu_{2-x}Fe_xSi_2$.[7]

Application of pressure to URu_2Si_2 induces a transition from the HO phase to a large moment AFM phase at a critical pressure $P_c \approx 1.5$ GPa.[3] Interestingly, substitution of smaller Fe ions for Ru in URu_2Si_2 induces a similar HO-AFM transition at a critical Fe concentration $x_c \approx 0.1$ (see Figure 1), an effect which has been attributed to "chemical pressure," owing to the reduction of the unit cell volume.[4,5] Single crystals of $URu_{2-x}Fe_xSi_2$ have been synthesized in our laboratory at UCSD,[5] and measurements of the electrical resistivity of these crystals under pressure revealed that chemical pressure and applied pressure are additive in driving the HO-AFM transition.[6] This suggests that $URu_{2-x}Fe_xSi_2$ may be used to study the HO and AFM phases at ambient pressure with techniques that cannot readily be performed on URu_2Si_2 under high pressure (e.g., angle resolved photoemission spectroscopy, scanning tunneling spectroscopy, neutron scattering at high pressure, etc.).

As an example, electrical resistivity measurements as a function of T on $URu_{2-x}Fe_xSi_2$ single crystals in magnetic fields H up to 45 T have been used to construct the 3D T–x–H phase diagram shown in Figure 2.[7] The surfaces represent the boundaries between the paramagnetic (PM), HO, AFM, and high-field ordered phases that emerge upon suppression of HO in high fields. These and other ambient pressure investigations of HO and AFM in $URu_{2-x}Fe_xSi_2$ single crystals will prove useful in developing an understanding of the underlying physics and, perhaps, even unmasking the identity of the elusive HO phase.

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Asymmetric Nuclear Matter under Extreme Condition

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Recent observation of the merging of two neutron stars gives us a glimpse of the properties of asymmetric compact nuclear objects under extreme conditions. The final fate of the two merging neutron stars is still unknown. Whether they merge into a black hole, or a giant neutron star or a transient neutron star that will collapse into a black hole depends on the equation of state (EOS) of nuclear matter. In a neutron star, the EOS is dominated by the symmetry energy, which describes the change in binding energy that arises from an imbalance in the number of neutrons and protons. The pressure driven by the symmetry energy counteracts the gravitational force, preventing the neutron star from collapsing into a black hole.

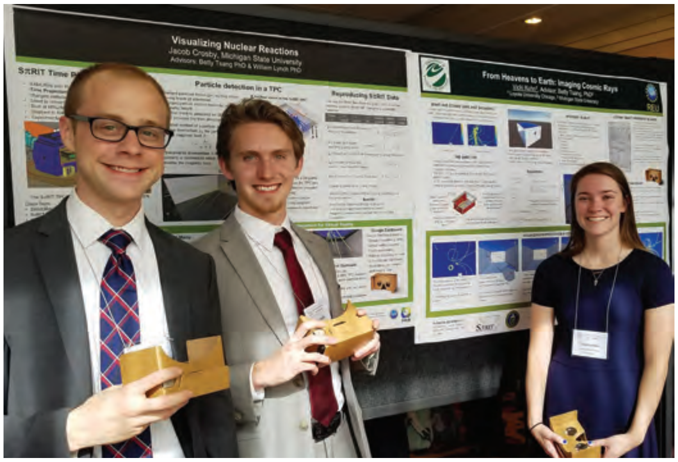

Figure 1. Cross-sections of 304L stainless produced via LENS, and a 3D reconstruction of TriBeam data. Grain orientations shown with inverse pole figure coloring.

Figure 2. PhD student Andrew Polonsky with the TriBeam.

A variety of experiments are needed to study the density dependence of the symmetry energy. At densities at and slightly above normal nuclear matter density, typical of nuclear interiors, we study heavy-ion collisions and fission processes at the National Superconducting Cyclotron Laboratory (NSCL). At twice nuclear matter density, which is more relevant to neutron star mergers, we compare charged-pion spectral ratios produced in collisions between neutron-rich and symmetric systems at RIKEN, Japan. In addition to supporting postdoctoral scholars, the current grant allows participation by graduate and undergraduate students, creating a pipeline for nuclear scientists, which is important to the Nation's Stockpile Stewardship Program.

A series of experiments to study the collisions of tin nuclei was completed in the spring of 2016 using the SpiRIT Time Projection Chamber (TPC). The results should allow us to put constraints on the symmetry energy at twice normal nuclear matter density. In the poster session of the April 2017 SSAP symposium in Chicago, Jon Barney, who is analyzing the TPC data for his thesis, received an outstanding poster award. The visual data that show artful tracks of cosmic showers as well as nuclear collisions have attracted a lot of interest among undergraduate students. At the 2017 Conference Experience for Undergraduates (CEU) in Pittsburgh, Pennsylvania, Jacob Crosby, an undergraduate student, and Vicky Kuhn, an REU (Research Experience for Undergraduate) student, presented their projects which used Google Cardboard virtual reality and augmented reality platform and a smart phone app to show nuclear collisions using data from the SpiRIT TPC (see Figure 1).

Experiments that will measure neutron and proton spectra to study the symmetry energy at low density are being prepared at Michigan State University (MSU). Figure 2 shows Kyle Brown, an SSAP postdoctoral researcher supported by this grant, on a ladder, testing the new charge-particle veto wall made of 23 1-cm-thick, 9.4-cm-wide, and 250-cm-long plastic scintillators installed in front of two neutron walls. The veto wall will identify charged particles from neutrons emitted in heavy ion collisions. Beam commissioning and calibration of the veto-wall/neutron wall combination started in December 2017. Two experiments are planned for February and March of 2018. The experiments will provide both the density and momentum dependence of the symmetry potential. Such information will help scientists to determine the density at which the neutron star crust ends and the core begins. MSU graduate and undergraduate students also work on this project.

Preparations for the experiment to measure fission barriers in the proton-rich lead region using the Active-Target TPC are underway. Beam identification is the main challenge of the experiment. We are building an ion chamber and two state-of-the-art channel-plate detectors to identify the beam using its energy loss, magnetic rigidity, and time-of-flight. This project is led by Kyle Brown who is the recipient of the 2017 Division of Nuclear Physics dissertation award.

New High Resolution Neutron Detector with Tracking (NEXT) – A New Approach to Neutron Detection

University of Tennessee, Knoxville ◆ PI: Robert Grzywacz (rgrzywac@utk.edu)

Improving the quality of fast neutron energy measurements in the 0.1-10 MeV range is one of the big challenges in experimental nuclear physics. The groups at the University of Tennessee (UTK) and Tennessee Technological University (TTU) are working on a new concept of a detector which will utilize a combination of recently developed technologies. The new detector called Neutron Detector with Tracking (NEXT) will complement and, in the future, supersede the Versatile Array for Neutron Detectors at Low-Energies (VANDLE). VANDLE, which is presently operating, was developed by the RIBSS consortium of universities funded by the Stewardship Science Academic Alliances program. The NEXT development team is led by Robert Grzywacz and Lawrence Heilbronn from UTK and Mustafa Rajabali from TTU.

The idea behind NEXT is to use the localization of the neutron interaction within the scintillating material to improve the neutron time-of-flight measurement. The ultimate goal is to build an array of detectors to be used at the new generation radioactive beam facilities such as FRIB and employ NEXT to measure neutrons emitted from unstable nuclei. The new detector may offer a dramatic improvement in detection sensitivity and will enable measurements of exotic nuclei that are very difficult to produce. Very neutron-rich nuclei will decay via beta decay and populate highly excited states in the daughter nucleus, which are likely to be neutron-unbound. Neutron spectroscopy will thus become a complementary or even dominant method of investigating beta decay of very neutron-rich nuclei. The high detection efficiency and excellent energy resolution that the NEXT detector will offer are critical for the future investigations of beta-delayed neutrons. The future measurements will address crucial nuclear structure challenges necessary to understand the properties of nuclei on the r-process nucleosynthesis path. The high neutron energy resolution will allow accurate measurement of excitation energy and decay widths of neutron resonances. While the detector is primarily developed for beta-delayed neutron spectroscopy, NEXT can also be used in direct reaction studies as well as in applied sciences where the neutron time-of-flight measurement requires compact, efficient neutron detection.

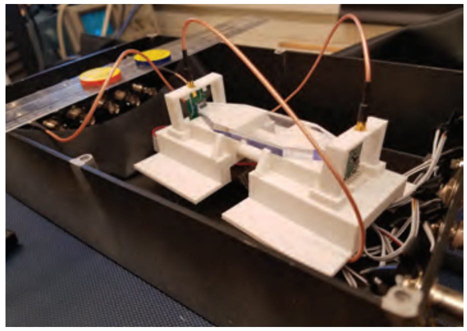

Figure 1. Prototype NEXT scintillator tile in the 3D printed frame with silicon photomultiplier readout on both ends.

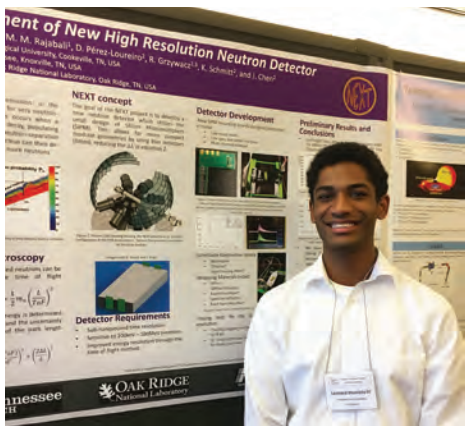

Figure 2. TTU student Leonard Mostella III presenting the NEXT project at the DNP meeting.

The detector will combine thin layers of neutron-gamma discriminating plastic scintillators which will be read out by very small but sensitive silicon photomultipliers and digital electronics. This will enable a highly compact design and allow millimeter resolution for the localization of the interaction point. This position resolution requires good timing resolution in the range of 200-300 picoseconds and a low energy threshold for neutron detection. These qualities will be combined within the new design.

A group of postdoctoral scholars and students is working on the design and prototyping. Drs. Kyle Schmitt (now LANL) and David Perez-Loureiro developed a Monte Carlo model needed to optimize the light collection and to simulate the detector performance. The electronic workshop at UTK produced a compact, linear array of silicon photomultipliers which is of crucial importance for the development of this detection system. A set of proof-of-principle measurements with various shapes of the detector modules and different reflective materials was carried out using radioactive sources. This work was the subject of the summer student project of Leonard D. Mostella from TTU. The use of novel 16-bit resolution digital electronics made it possible to improve the digital timing algorithm for silicon photomultiplier signals. In the Fall of 2017, UTK graduate student Joseph Heideman joined this project. He is working on the proof-of-principle time-of-flight measurement with single-layered prototype detectors. The next step in development involves the construction of multi-layered system and development of tracking and neutron-gamma discrimination algorithms.

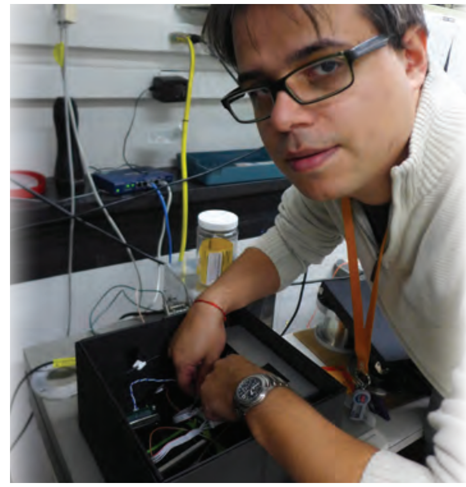

Figure 3. Dr. David Perez-Lureiro preparing the NEXT prototype measurement in the light-tight test enclosure.

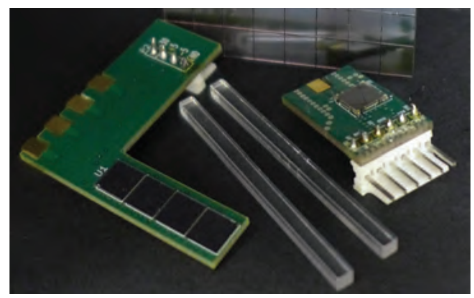

Figure 4. Essential components of the NEXT detector: silicon photomultiplier arrays and scintillator segments.

Robust Extractive Scintillating Resin and Adsorptive Membranes for Plutonium Isotopic Analyses of Aqueous Media

Clemson University, [1]Environmental Engineering and Earth Sciences , [2]Chemical and Biomolecular ◆ PI: Timothy A. DeVol[1], devol@clemson.edu
Co-PIs: Scott M Husson[2] and Brian A. Powell[1]

The objective of this research is to advance scientific understanding in the development of high-selectivity sensor materials and high-sensitivity sensors for ultra-trace-level isotopic analysis of plutonium in aqueous media. The capability brought about by this research program, to concentrate and quantify plutonium in natural water, will be a powerful nuclear forensics tool that is currently not available. The two-prong approach involves the design, synthesis, and characterization of a new class of extractive scintillator resins for rapid on-line quantification, and sorptive membranes for direct quantification of plutonium isotopes using alpha spectroscopy. Understanding the chemistry of plutonium in a natural water is imperative to development of the proper sensor. Three material platforms were developed to identify a suitable ligand for Pu(IV) and Pu(V): 1) polyaniline-hallosite nanocomposites (PANI-HNT), 2) derivatives of N, N, N', N' tetraalkyldiglycolamide (DGA), and 3) scintillator-modified commercial extractant resin.

Polyaniline is a versatile polymer with properties that depend on the redox state and doping condition. PANI doped with toluene sulphonic acid (TSA) and two derivatives of PANI with additional oxygen bearing functional groups (PANI-m1 and PANI-m2) were studied. Template polymerization of the PANI derivatives on halloysite nanotubes (HNT), a natural multilayered aluminosilicate mineral, yielded nanostructured Pu sorbent materials. Control samples also were prepared without any template. Figure 1 shows transmission electron microscopy images of pure nanotubes and PANI(TSA), PANI-m1 composites. We demonstrated that PANI with HNT has a synergistic effect on the performance of the material as a sorbent (Figure 1 insert). Future work will enhance selectivity of such nanocomposites through chemical design of the PANI shell.

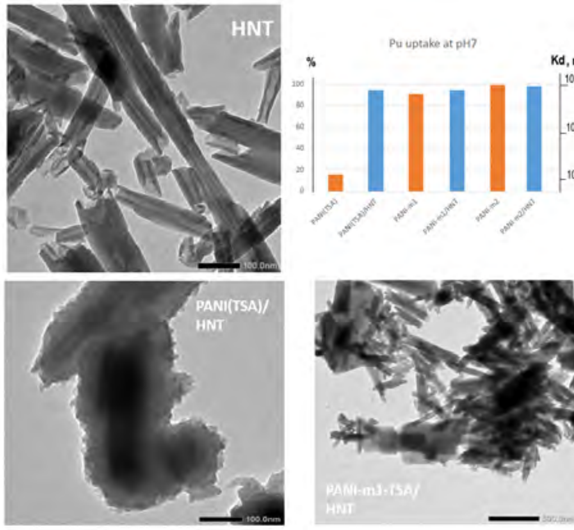

Figure 1. TEM images of HNT and HNT/PANI nanocomposites (scale bar is 100 nm for HNT and PANI(TSA)/HNT images and 500 nm for PANI-m1-TSA/ HNT image). Top right shows ^{242}Pu uptake by PANI nanocomposites from 6946 Bq/mL aqueous solution at pH7 and corresponding K_d values (right axis).

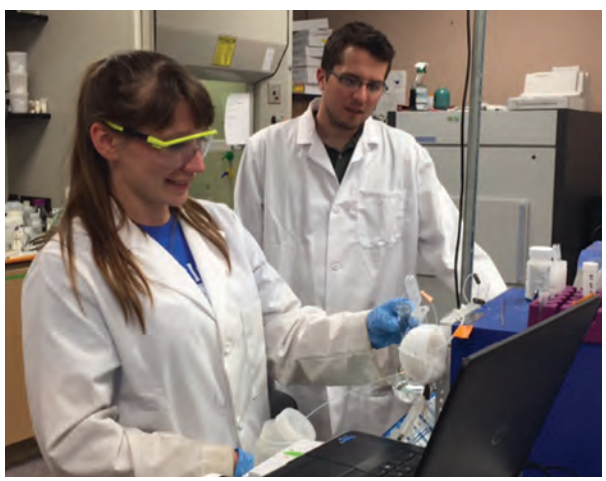

Figure 2. Kamila Kołacińska, Fulbright Scholar, instructing William Fullmer, MS student, on the operation of the flow injection analysis system used to characterize Pu sorbents.

Diglycolamide (DGA) derivatives are promising for the recovery of actinides from acid solutions. Highly stable DGA extractive resins can be prepared using two approaches: 1) synthesize DGA monomers that can be suspension copolymerized with other styrene based and organic fluor monomers, and 2) react a DGE derivative onto pre-formed poly(styrene-co-chloromethylstyrene) resin. Four alkyl-substituted DGA compounds, N,N,N′,N′-tetraisobutyl diglycolamide (TiBDGA), tetrapropyl-DGA (TPDGA), tetrahexyl-DGA (THDGA), dipropyldimethyl-DGA (DPDM-DGA) and their corresponding monomer forms vTiBDGA, vTPDGA, vTHDGA, and APDM-DGA were synthesized. Tetraethyl-DGA (TEDGA), tetrabutyl-DGA (TBDGA), and tetraoctyl-DGA (TODGA) also were synthesized. Liquid-liquid extraction of ^{242}Pu demonstrated that TiBDGA and TBDGA extracted > 99.5% of Pu(IV) ions from 2 M HCl comparing to 62% for TODGA and 53% for THDGA. TiBDGA, TBDGA, TODGA, and THDGA all extracted > 93 % of Pu from 3 M HNO3. These results reveal that TiBDGA and TBDGA are ideal extractants for sensor applications since they have a high selectivity at low acid concentration and transparent appearance, which is important to avoid color quenching during scintillation detection. Future work will fabricate extractive resins by copolymerization of the four novel DGA monomers with other styrenic monomers.

Pu-02 Analig® is a proprietary silica-based resin developed by IBC Advanced Technologies® for selective aqueous Pu uptake. We attached a plastic scintillator to the surface of this material, referred to as S-Pu-02. Batch uptake tests indicated high affinity (K_d of 1,780 ml/g) for ^{242}Pu(IV) from pH 1 solution. The S-Pu-02 resin subsequently was loaded into a PTFE column, and detection efficiency was quantified with a liquid scintillation counter without the introduction of liquid scintillation cocktail. The absolute detection efficiency was 36.4%, demonstrating the radioluminescent properties of S-Pu-02. Future work will determine the role of competing ions and optimizing detection efficiency for the sensor.

Kay Kolos, Lawrence Livermore National Laboratory (karolina.kolos@gmail.com)

Years at LLNL: 2015 to Present ◆ Degree: PhD, Physics ◆ SSAA Program: 2014-2015, University of Tennessee

After obtaining my PhD in 2012, I moved to Knoxville, TN, and started my postdoctoral appointment at the University of Tennessee at Knoxville (UTK) with Professor Robert Grzywacz. The focus of my research at UTK was to study the structure and decay properties of atomic nuclei far from stability using radioactive ion beams of fission fragments. When uranium or another actinide fissions, neutron-rich fragments unstable to β decay are released. In the β decay of these radioactive isotopes, the resulting nucleus can be left in such a highly-excited state that they can subsequently emit a neutron. A detailed understanding of this decay mode is necessary to determine the properties of neutron-rich isotopes. This knowledge will help to clarify how the elements from iron to uranium are produced in astrophysical environments, and predict the performance of nuclear reactor designs.

The Stewardship Science Academic Alliances (SSAA) Center of Excellence for Radioactive Ion Beam Studies for Stewardship Science, led by Professor Jolie Cizewski, supported the development of the Versatile Array of Neutron Detectors at Low Energy (VANDLE) (see Figure 1). This detector is now utilized to measure β-delayed neutrons to help us understand the details of this decay process and structure properties of the short-lived fission products. During my almost three-year appointment at UTK, when I was supported in part by the Center, I had a chance to be a part of various experiments at different user facilities: the National Superconducting Cyclotron Laboratory, Argonne National Laboratory (ANL), and ISOLDE (CERN, Geneva). It was a great opportunity for me to not only travel and learn about other laboratories in the United States, but also to collaborate with other scientists and students who are a part of the NNSA complex. I participated in the SSAA meetings and Center workshops held at Los Alamos and Lawrence Livermore National Laboratories (LLNL). It was during these meetings that I had a chance to learn in detail about the work that NNSA supports, and the importance of nuclear physics studies to national security and stockpile stewardship. I became interested in practical applications of nuclear science and decided to apply for a job at LLNL with Dr. Nicholas Scielzo, who focuses on low-energy nuclear physics and decay studies.

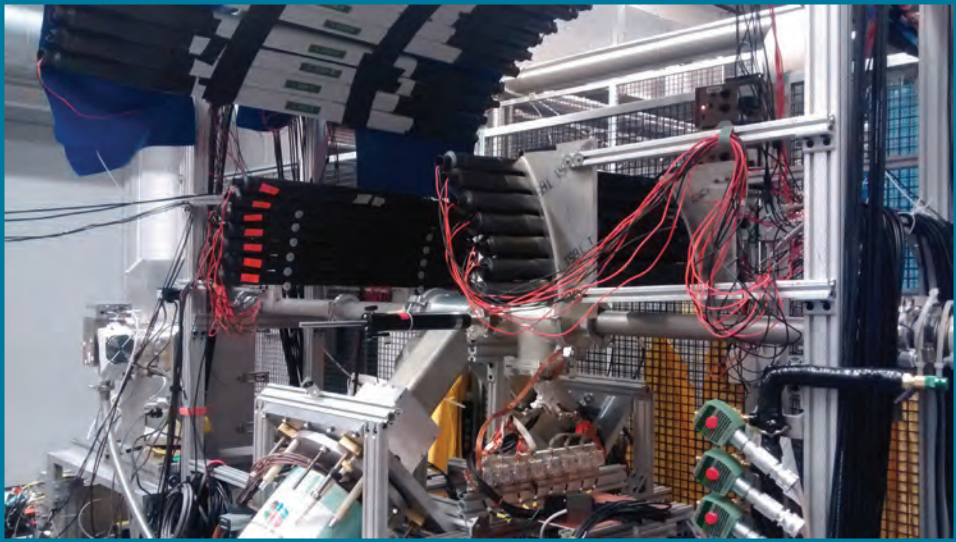

Figure 1. Photograph of the VANDLE set up at Argonne National Laboratory. The VANDLE bars are made of plastic and are equipped with photomultiplier tubes at each end. Also shown are the mounts for high purity Ge (HPGe) gamma-ray detectors. The beam enters from the right to implant radioactive species on a moveable mylar tape surrounded by four thin beta-particle detectors.

My current research at LLNL concentrates on precision measurements of the γ-ray intensities that play a crucial role in science-based stockpile stewardship and nuclear forensics. One of the most straightforward and reliable ways to determine the number of fissions that occurred in a chain reaction is via the detection of the characteristic γ rays emitted during the β decay of the fission product. These γ rays are emitted in only a fraction of the decays, and this fraction (the γ-ray branching ratio) must be known accurately to determine the total number of nuclei that undergo fission. Even though most of the long-lived fission products have already been measured, some of the nuclear data currently available has large (up to 30%) uncertainties. In our experiment, we intend to achieve a precision of 1-2%. We produce high-purity sources at the CARIBU fission fragment facility at ANL by implanting radioactive ions on thin carbon foil backings. The sample is then shipped to Texas A&M University and inserted into the center of a windowless 4π β gas proportional counter for β detection. The γ rays are counted using a HPGe detector that has been painstakingly calibrated, to 0.2% over 50-1,500 keV energy range, by Professor John Hardy's group at Texas A&M. The branching ratio is obtained using the ratio of detected β-γ coincidences and total β counts (total disintegrations). This work has been very challenging and exciting at the same time. It gives me an opportunity to participate in every step of the measurement and keeps me inspired to continue my research in the field of nuclear physics as applied to stewardship science.

Anirban Mandal, Los Alamos National Laboratory (anirban.mandal@lanl.gov)

Years at LANL: 2017 to Present ◆ Degree: PhD, Mechanical Engineering ◆ SSAA Program: 2010-2016, Washington State University

I was introduced to the fascinating world of experimental shock wave research while pursuing my PhD at the Institute for Shock Physics (ISP)—a SSAA supported Center of Excellence— at Washington State University (WSU). The world-class experimental capabilities, knowledgeable and helpful research staff, and the opportunity to learn from Prof. Yogendra Gupta (my PhD advisor) at ISP were the key factors in choosing WSU. Support from the SSAA program allowed me to undertake rigorous doctoral research to examine, both experimentally and computationally, the elastic-plastic deformation of shock compressed Molybdenum (Mo) single crystals. Molybdenum, a body-centered cubic (BCC) crystal, is important for nuclear reactors and other applications due to its high strength and superior heat- and corrosion-resistant properties. Under dynamic loading, BCC metal crystals exhibit a plastic response that is more complex, far less understood, and relatively less studied compared to the plastic response of metals with close-packed structure (e.g. face-centered cubic and hexagonal close-packed). My work showed that the deformation response of shock compressed Mo single crystals is both time-dependent and highly anisotropic (see Figure 1). It was demonstrated that the shear stresses on operative slip systems, and not the longitudinal stresses, at the elastic limit are a better measure of the material strength for anisotropic solids. The operative slip systems were identified and the effect of the large Peierls stress of screw dislocations on the deformation response was highlighted. Overall, my work has provided comprehensive and new insights into shock-induced plasticity of BCC single crystals, including the development of a crystal plasticity-based continuum model. By presenting my work at APS shock conferences and SSAP annual symposiums, I received valuable feedback from attendees. The skills and knowledge acquired during my graduate education, including the strong emphasis on rigorous learning and independent thinking at the ISP, helped me grow as an independent researcher and led to my current position at Los Alamos National Laboratory (LANL).

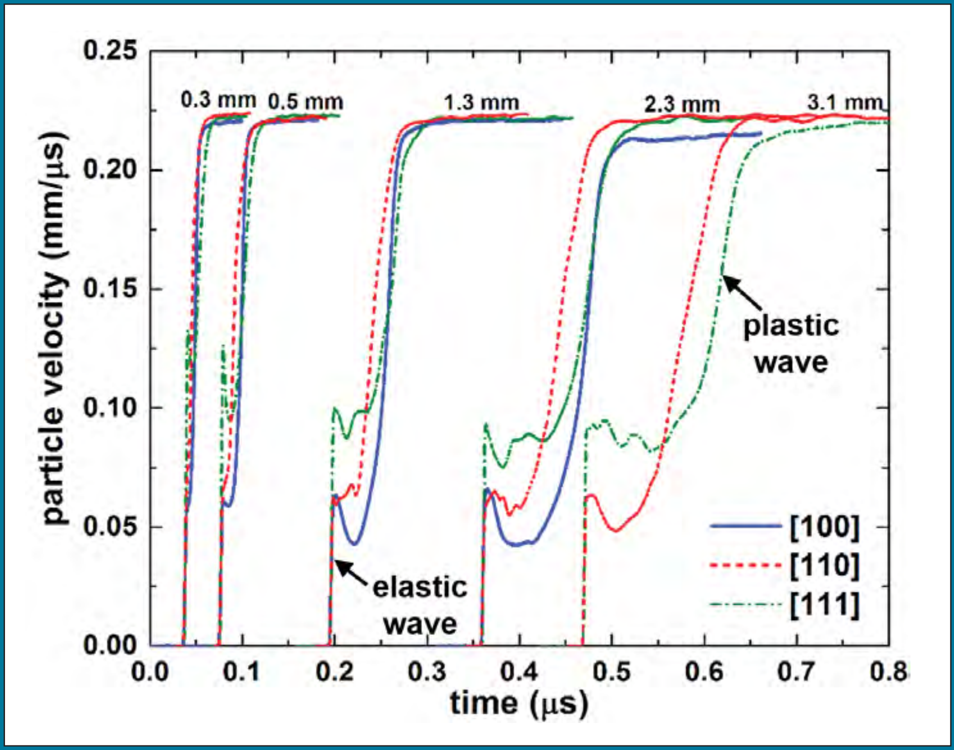

Figure 1. Elastic-plastic wave profiles measured at different propagation distances in [100], [110], and [111]-oriented Mo single crystals suggest a time-dependent and highly anisotropic material response under shock wave loading.

As a LANL postdoc located at the Dynamic Compression Sector (DCS)/ Advanced Photon Source (APS), I have the unique opportunity to work with and learn from both the shock wave and the x-ray scientists. At DCS, I am using a propagation-based x-ray phase contrast imaging (PCI) technique, along with x-ray diffraction to examine shock compaction of porous, granular systems. Unlike traditional methods (laser velocimetry and post-shock microstructural analysis of recovered samples), which provide limited and indirect information, x-ray PCI permits in situ, real-time examination of material response with micron spatial resolution. A detailed analysis of the x-ray images will provide new insights into the compaction response and will help develop improved material models for granular materials. Being stationed at APS has also allowed me to learn about the different sectors and the various x-ray techniques used to conduct research at these sectors. My research work at DCS is contributing strongly to LANL's scientific and programmatic missions, and the overall experience is extremely valuable for my growth as an early-career scientist.

During my PhD I was fortunate to interact with and learn from many scientists from the DOE/NNSA laboratories, academia, and industry during their visits to the ISP (for reviews and seminars), and interactions at shock conferences and SSAP annual symposiums. Some personal highlights have been learning about the Z machine at Sandia National Laboratories and the National Ignition Facility at Lawrence Livermore National Laboratory, attending Dr. Donald Cook's talk on the U.S. nuclear deterrence program, and discussing my work with many distinguished visitors. These enriching experiences, made possible by my SSAA supported studies, have provided me with a broad and valuable perspective on scientific research and responsibilities.

Jeffrey M. Montgomery, Lawrence Livermore National Laboratory (montgomery35@llnl.gov)

Years at LLNL: 2015 to Present ◆ Degree: PhD, Physics ◆ SSGF Program: 2010-2012, University of Alabama, Birmingham

I began my work with the SSAA program in 2010 at the University of Alabama at Birmingham. While working with Dr. Yogesh Vohra, I studied phase transitions in metals at static high pressures generated in a diamond anvil cell (DAC). My thesis work centered around the production and use of new types of diamond anvils that can be manufactured via chemical vapor deposition (CVD) growth of additional diamond material on top of natural diamond anvils.

My primary project was the creation of the first "self-heating" boron-doped diamond anvils.[1] These consist of normal diamond anvils with a thin, electrically conducting homoepitaxial layer of CVD-grown boron-doped diamond surrounding the outer portions of the anvil. By applying an electrical current while monitoring the anvil temperature with an attached thermocouple, these anvils allow the precise control of the temperature of the high-pressure environment without heating the rest of the DAC. This allows for relatively rapid changes in sample temperature compared to other resistive heating methods, and more precise control at low-temperatures than laser-heating techniques. I used the first of these anvils to study the hexagonal structures of gadolinium to 8 GPa and 600 K, but the difficulty of producing these boron-doped anvils limited my PhD experiments to single-sided heating geometries.

My second project was the testing of two-stage diamond micro-anvils[2] also grown by CVD. These anvils contain a "second stage" consisting of tiny secondary anvils grown on the culets of natural diamonds. Because the second stage is grown directly on the natural anvils, these anvils do not suffer from the problems with alignment and repeatability of designs using freely-sliding second stages. I used the first generation of these anvils to study lutetium and to develop the capability of collecting and analyzing two-dimensional x-ray diffraction scans of these micro-anvils.

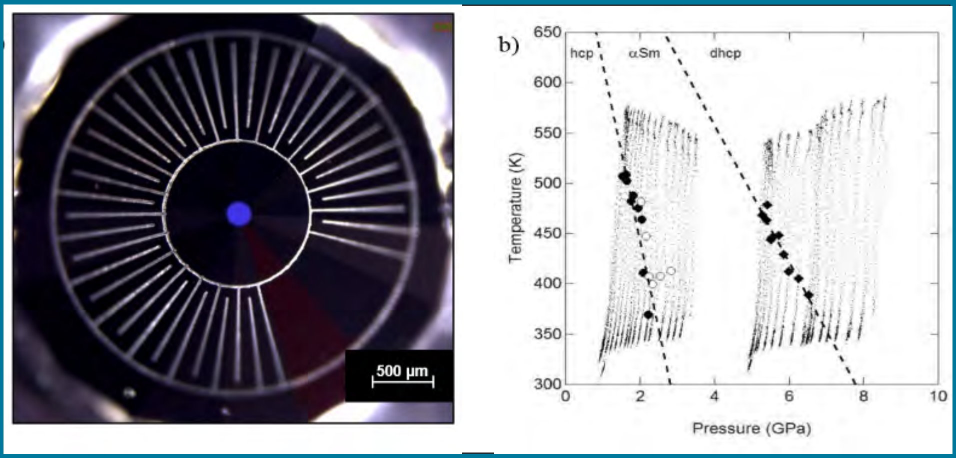

Figure 1. (a) A tungsten-sputtered self-heating diamond anvil with patterned heating circuit. (b) The phase diagram of gadolinium scanned with a boron-doped heater anvil. Dots represent points where the crystal structure was measured, and open and closed symbols are where phase transitions were observed either by anomalous changes in sample volume (filled symbols) or discontinuities in the x-ray intensity (open symbols). Proposed phase boundaries are drawn with dotted lines.

Every aspect of my work has benefitted from my time in the SSAA program, and my post-doctoral work is a direct extension of the work I did under the SSAA. After finishing my PhD, I was hired by Lawrence Livermore National Laboratory to further develop self-heating diamonds. The new design (see Figure 1) consists of a normal anvil that has been sputtered with tungsten, and then patterned with a heating element via laser machining. This design is easier to make than its predecessor, and allows pairs of anvils to be easily produced for double-sided heating geometries needed to get to higher temperatures and to create hydrostatic high-pressure environments with low thermal gradients.

In addition to fabricating and testing the new heating anvils, my work also includes the development of precise and reliable control systems to procedurally drive the heating current, measure the temperature, and control the sample pressure all while collecting Raman scattering information or x-ray diffraction information at synchrotron. Since these experiments can yield hundreds of thousands of spectra in as little as an hour of collection time, I also am developing new tools for the analysis of these large data sets.

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High Energy Density Laboratory Plasmas

Inverse Skin Effects in Pulsed-power Driven Plasmas

Cornell University ◆ PI: John Greenly, jbg2@cornell.edu

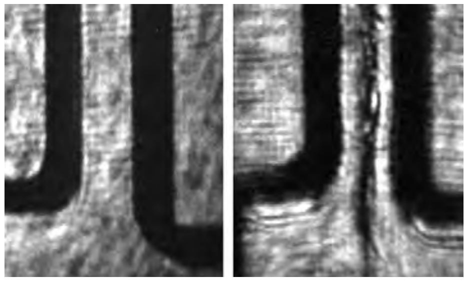


Figure 1. Shadowgraphs of the gap between a pair of parallel plates, self-magnetically insulated electrodes carrying current to a wire load (above the image frame).

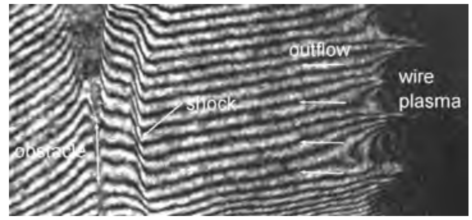


Figure 2. interferometry of a standing bow shock produced by placing an obstacle in the outflow from a (sausage-unstable) plasma column formed from a single aluminum wire carrying 800 kA.

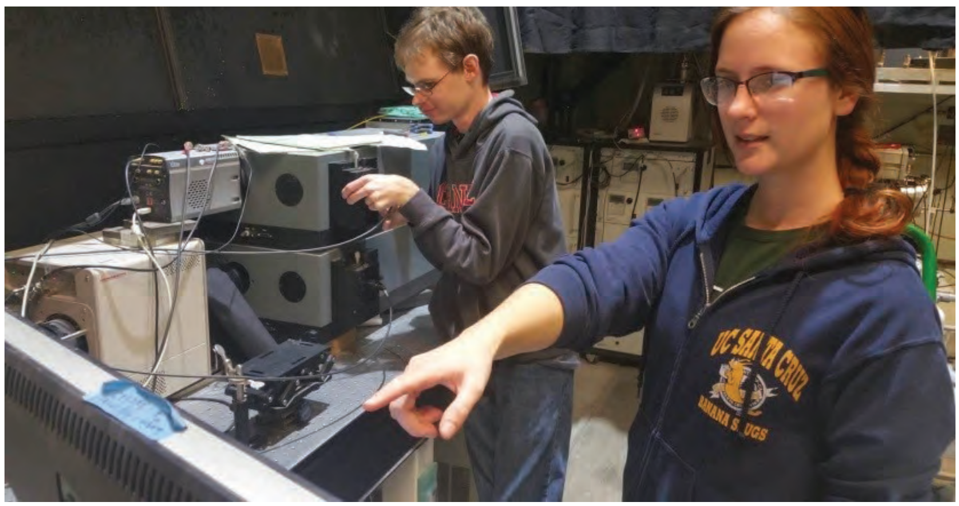


Figure 3. Graduate students Sophia Rocco and Jacob Banasek setting up the spectroscopy.

The skin effect, the finite rate of penetration of pulsed current and magnetic field into a conductor, is a simple diffusive process in a rigid conductor but, in a fluid conducting medium like plasma, Alfven long ago pointed out that skin effects become quite complex as the medium moves in response to magnetic pressure gradients.

We are studying the response of current-carrying plasma to a rapid reversal of electric field imposed at its boundary. An applied pulsed voltage drives rising current; the current density J and magnetic field B diffuse into the column while the magnetic pressure gradient (JxB force) accelerates the plasma, as for example in an imploding Z-pinch. If the driving voltage is quickly reversed, B must begin to decrease outside the plasma but this decrease cannot immediately penetrate the plasma, so a reversed current is driven at the plasma boundary. The reversed JxB force on this outer layer accelerates it outward, away from the body of the plasma. These effects, which Alfven called the inverse skin effect, can result from a reduction of current driven by either a changing applied electric field E, or by the vxB term in Ohm's law, J=σ(E+vxB), acting on times shorter than the diffusive penetration time of the plasma.

We are studying this phenomenon in plasmas produced by a variety of loads driven by our COBRA 1 MA, 100-200 ns pulsed power driver at Cornell. We do indeed see outflows driven by the inverse skin effect that initiate exactly at the time of voltage reversal after peak current. The most basic observation, in both experiments and in simulations with our PERSEUS extended MHD code, is that the density of these outflows is quite low, of order $10^{17}/cm^3$ or less, far below the density of the high energy density core plasmas from which they come. Nevertheless, these outflows can carry high current densities and support large magnetic pressure gradients as they accelerate. They can significantly influence the dynamics of the high energy density core plasma, and change its coupling to the driving power source.

The figures illustrate two examples of outflows we are studying. Figure 1 shows shadowgraphs (an optical method using refraction that reveals non-uniformities in transparent media) of the gap between a pair of parallel plates, self-magnetically insulated electrodes carrying current to a wire load (above the image frame). During current rise, the wire plasma produces intense XUV radiation that generates dense plasma confined on the electrode surfaces, as seen in the first shadowgraph 10 ns before voltage reversal, 20 ns after reversal (second shadowgraph). This plasma has been accelerated away from the surfaces, colliding in the middle of the 2-mm gap, despite very strong self-magnetic insulation with 1 MA current. Simulations show similar behavior, but only when the Hall term in extended MHD is included. Hall effects in plasma arise at relatively low density when electrons and ions decouple and move separately. This plasma gap closure can cause current loss, interfering with power coupling to the load.

Figure 2 shows interferometry of a standing bow shock produced by placing an obstacle in the outflow from a (sausage-unstable) plasma column formed from a single aluminum wire carrying 800 kA. The outflow density falls below $10^{17}/cm^3$ a few mm outside the opaque, dense plasma boundary. The density behind the shock front is ~$10^{18}/cm^3$.

We are presently using Thomson scattering of our 10 J, 3 ns 527 nm laser to diagnose these plasma flows. The photo (see Figure 3) is of graduate students Sophia Rocco and Jacob Banasek setting up the spectroscopy. Outflow velocity of 100 km/s is measured near a wire plasma column, but the low outflow densities present a real challenge requiring optimization of the diagnostic capability.

Continuation of the Application of Kinetic Simulations to Laser and Electron Transport Through High-Energy-Density Laboratory Plasmas

University of California, Los Angeles ◆ PI: Warren B. Mori (mori@physics.ucla.edu) ◆ Co-PI: Frank S. Tsung (tsung@physics.ucla.edu)

The University of California, Los Angeles (UCLA) Simulation of Plasmas Group has been supported by the NNSA to carry out research on laser and energetic particle transport in high energy density laboratory plasmas (HEDLP). These processes are fundamental research topics in the area of the nonlinear optics of plasma (NLOP), as well as being directly relevant to inertial fusion energy (IFE). The group's activities include developing software for studying HEDLP that run effectively on the largest computers in the world. The group is home to the Particle-in-Cell and Kinetic Simulation Software Center (PICKSC) http://picksc.idre.ucla.edu and all of its research activities and group members are listed on this web page. Through PICKSC, the group also makes its software available to researchers worldwide, including those at NNSA laboratories. The study of NLOP, as well as advanced computing, attracts talented graduate students and post-doctoral researchers.

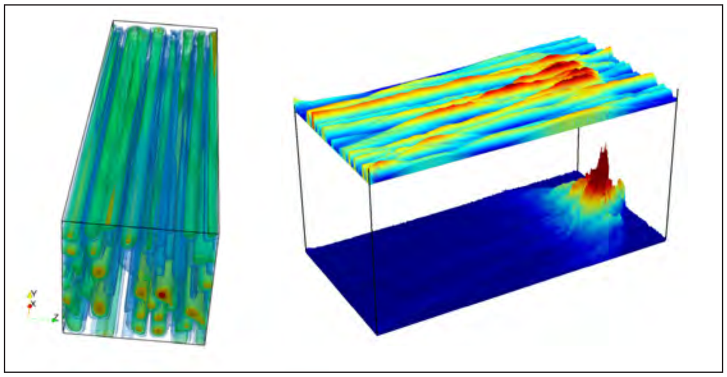


Figure 1. (left) 3D laser speckle pattern generated by random phase plate from the PIC code OSIRIS; (right) snapshots of the longitudinal electricl field (top) and the transverse electric field (bottom) from a 2D multi-speckle OSIRIS simulation. Our simulations showed that both external magnetic fields and temporal bandwidth can suppress SRS in IFE plasmas.

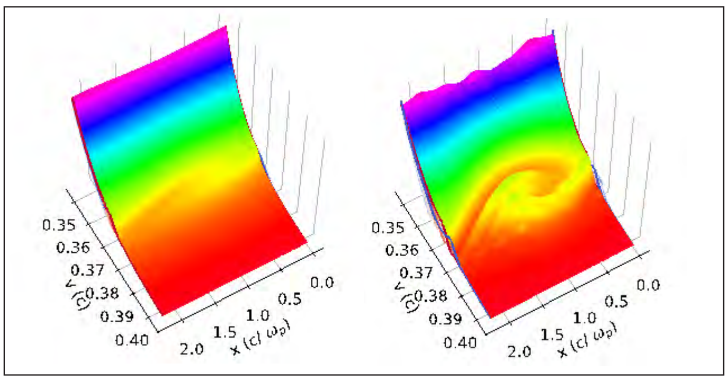


Figure 2. Steady-state phase space of weakly-collisional, driven, non-linear plasma waves. (a) When driven with a low amplitude, the plasma wave saturates such that the final state is almost Maxwellian. (b) When the driver amplitude is increased, a vortex begins to form signifying particle trapping. However, the phase-space reaches a steady state here because particle trapping does not proceed further due to self-collisions.

NLOP is both fundamental by nature and important to laser driven IFE, where it is imperative that laser light reaches where it is aimed when it is needed. An HED plasma can scatter, reflect, and bend laser light, and it can transfer the laser energy into energetic electrons through a number of laser plasma instabilities such as stimulated Raman scattering (SRS) and two-plasmon decay. In SRS the laser becomes a backscattered laser and a plasma wave, and in two plasmon decay it becomes two plasma waves. These are extremely complicated processes because they involve waves coupling to other waves, particles surfing on waves, and highly dispersive waves propagating in non-uniform plasmas. Furthermore, collisions can also have subtle effects on NLOP, despite the fact that collisions in HED plasmas are infrequent compared to the wave frequencies. Due to the complexity of all these interactions, computer simulations that follow the individual particle trajectories are necessary.

An HED plasma can be full of light waves, electron plasma waves, ion acoustic waves, and plasmas which are far from equilibrium with non-Maxwellian distribution functions. NLOP is further complicated by beam "smoothing" techniques that lead to large laser beams being broken up into smaller speckles that can move around in time and/or be shut on or off in time. If speckles are moved around or turned on and off quickly enough, it may be possible to greatly reduce the occurrence of NLOP processes. The need to consider the interaction of many speckles also differentiates the NLOP from the nonlinear optics of traditional materials. Over the years we have carefully studied isolated aspects of these processes and studied how a few speckles interact.

Recently, the interactions of many speckles and the effect of magnetic fields have become topics of study. We have modified our software (our code OSIRIS) to permit many speckled laser beams, including bandwidth and on/off cycles (STUD pulses), which allows the speckles to move around in time. In Figure 1 (left) we show an example speckle pattern generated by OSIRIS in three-dimensional (3D). Also shown are the results (right) of a 2D simulation run long enough (3 picoseconds) to see a speckled laser beam undergoing SRS for NIF-relevant laser and plasma parameters. It has been found that with sufficient bandwidth, SRS could be significantly reduced.

An important aspect of HED plasmas is that they require both continuum and discrete descriptions. This can be seen by examining the number of electrons within a Debye sphere: $(4\square/3)\, n\lambda_D^3 = 2.1\times10^3\, (T_{KeV})^2/(P_{MBar})^{1/2}$. At high energy densities (pressures) this parameter is not necessarily large, meaning that discrete particle effects and collisions cannot be ignored. The UCLA Simulation of Plasmas Group has a suite of software tools to study the behavior of HED plasmas from various points of view, including particle-in-cell codes that can include collisions and a Vlasov-Fokker-Planck (VFP) code. This is very instructive for graduate students and post-docs. Figure 2 shows a recent example from our open source (on GitHub) VFP code OSHUN in which it was found that driven nonlinear electron plasma waves can reach a nonlinear steady state in the presence of collisions.

Line Emission from High-Z Multiply Ionized Ions Influenced by Dielectronic Recombination and Polarization*

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

The Report of the 2009 Workshop on Basic Research Needs for High-Energy-Density Laboratory Physics recognized the vital importance of High-Z, Multiply Ionized High Energy Density (HED) Atomic Physics for High Energy Density Laboratory Plasma (HEDLP) Science. This report emphasized that—

"The complicated nature of high-Z atoms at extreme densities makes their atomic physics and application to HEDLP a unique and complex sub-discipline. Achieving an understanding of high-Z atomic physics is essential to designing "well-posed" HEDLP experiments and diagnostic instruments, and to analyzing the data obtained from them. This is equally true of HED plasmas produced by lasers, pulsed-power machines and intense heavy-ion beams."

Figure 1. UNR research team assembling and adjusting the x-ray spectrometer/spectropolarimeter for HEDLP experiments. In front, clockwise, beginning far right: Matt Cooper, Veronica Shlyaptseva, Emil Petkov, Kim Schultz, Ishor Shrestha, and Austin Stafford.

The HEDLP grant within the SSAP program provides us with an excellent opportunity to study high-atomic-number Z multiply ionized ions in high energy density HEDP as we seek to calculate and validate atomic properties and spectra of such ions as a function of plasma parameters and electron distribution functions. The areas of our particular interests are the research on polarization of x-ray line emission from these multi-charge ions, and the study of dielectronic recombination, an important process for astrophysical problems and HEDLP, as well as the associated satellite lines, frequently used for plasma diagnostics. While the current grant is for three years, a total of four faculty, two research scientists, two postdoctoral researchers, 16 graduate, and six undergraduate students have been supported by NNSA programs in a little more than a decade. In 2017, five graduate students, two research scientists, and two research faculty were involved in this HEDLP research. Our graduated PhD students are working at Sandia National Laboratories, Lawrence Livermore National Laboratory (LLNL), the Naval Research Laboratory, Naval Air Warfare Center, and UNR.

Our HEDLP project that started in October 2015 focuses on the comprehensive experimental and theoretical study of line emission from multiply ionized high-Z ions produced in z-pinch plasmas and benchmarked with LLNL Electron Beam Ion Trap (EBIT) data. The spectral range of interest between 3 and 8 Å included L-shell Mo and Ag and M-shell W spectra. Since then, we have made substantial progress in studying line emission from the above-mentioned ions influenced by dielectronic recombination and polarization. For example, we were able to perform the first measurements of x-ray line polarization of Ne-like Mo ions both at the LLNL EBIT and in pulsed power plasmas. A very important component in the success of studies of line polarization in plasmas is the ability to benchmark theoretical codes and calculations with line polarization data that are produced under-well controlled conditions, which was accomplished using the LLNL EBIT. Specifically, x-ray line polarization of several intense Ne-like Mo lines as a function of electron beam energy ranging from 2.75 to 15 keV at LLNL EBIT-I was measured for the first time and analyzed. Dielectronic recombination of L-shell Mo ions has been studied in detail also using the LLNL EBIT-1, but by modifying an electron distribution function to produce resonances. Comparisons between the theory and experiment show good agreement for relatively low (<850 eV) and high (>2 keV) electron beam energies. We have designed, manufactured, and successfully tested an x-ray spectrometer/polarimeter for HEDLP experiments. Using such a device with two identical α-quartz crystals (2d = 6.67 Å) to maximize polarization, we were able to measure x-ray line polarization of the Ne-like Mo lines in Z-pinch plasmas at NTF Zebra facility at UNR. Non-LTE modeling and various relativistic atomic physics codes are used to analyze L-shell spectra and x-ray line polarization of Mo ions. This study represents the first measurements of x-ray line polarization in Mo HED plasmas.

Collaborators

E.E. Petkov, A. Stafford, R. Childers, V.V. Shlyaptseva, I.K. Shrestha, M.C. Cooper, K.A. Schultz, C.J. Butcher (UNR), P. Beiersdorfer, N. Hell, G.V. Brown (LLNL).

Christine Krauland, General Atomics (kraulandc@fusion.gat.com)

Years at GA: 2016 to Present ◆ Degree: PhD, Applied Physics ◆ SSAA Program: 2007-2013 (graduate),University of Michigan; 2014-2016, University of California, San Diego

Over the course of my early career in high energy density (HED) science, I have had the great benefit of being supported by multiple avenues within the SSAP Program. My introduction to HED physics came through an undergraduate research opportunity program at the University of Michigan during my sophomore year when I joined Prof. Paul Drake's lab. Supported by SSAP, his research lab cultivated an environment for both undergraduate and graduate students to explore different facets of HED physics research, so it was an easy decision and great opportunity for me to stay under Prof. Drake's mentorship while I pursued my PhD in the field. During those studies, my primary focus was developing a new experimental platform at the Omega Laser Facility at the University of Rochester's Laboratory for Laser Energetics (LLE) to create and image radiative shockwaves similar to those occurring in astrophysical systems. This work was done specifically through the HED Laboratory Plasmas (HEDLP) award to University of Michigan for the Center for Laser Experimental Astrophysical Research with facility time at LLE made possible by support from the National Laser Users' Facility (NLUF) program. As a graduate student, I gained valuable knowledge in being able to design and lead several experiments at this large-scale laser facility where I implemented many different x-ray diagnostic techniques.

With this experience, I joined University of California, San Diego Prof. Farhat Beg's group for a post-doctoral fellowship as a lead on experimental campaigns at Omega EP and other smaller laser facilities, the former of which was again funded through the NLUF program. The majority of this work concentrated on hot electron generation and transport relevant to alternative ICF schemes. While the subject was in a different area under the HED science umbrella, the x-ray diagnostics were the same. My interest and understanding grew significantly as I worked to optimize design for x-ray imaging and x-ray spectroscopic techniques that would provide detailed information on our plasma conditions and electron beam profile created by high intensity laser interactions with target materials.

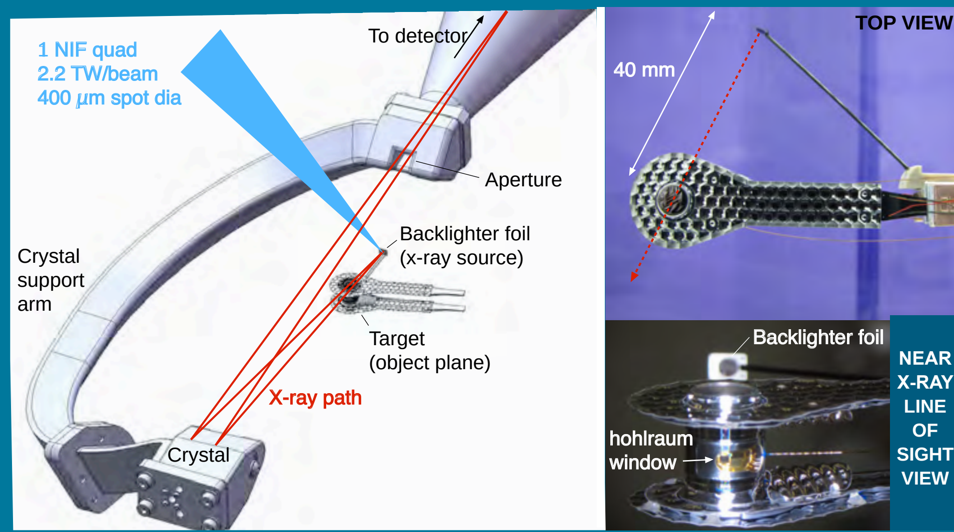


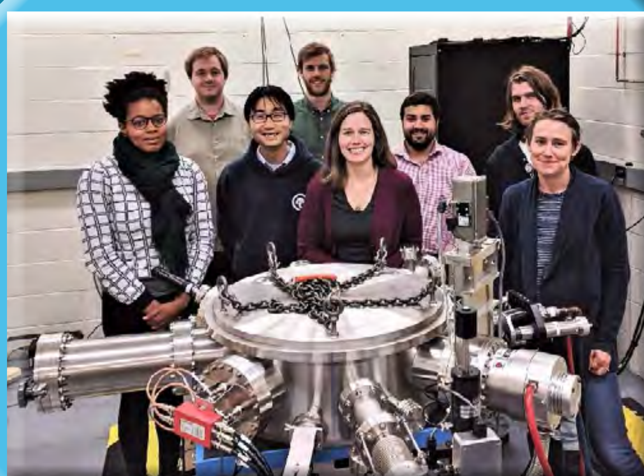
Figure 1. (Left) Schematic of the Crystal Backlighter Imager (CBI) diagnostic. A single NIF quad (i.e., 4 NIF beams) is used to irradiate a backlighter foil to generate x-rays used to image the main target. In the CBI scheme, these x-rays pass through the object to a spherically-bent crystal, designed specifically to Bragg reflect the primary x-ray line emission at near-normal incidence such that it passed back through a small aperture to a detector. This technique is a unique challenge in the NIF chamber as it requires the crystal and the detector to be on opposite sides of the target. Not shown in the cartoon are the other 188 NIF beams that indirectly drive the ICF capsule implosion. The CBI design limits the self-emission from the capsule as it implodes due to the narrow pass of the crystal that relays the image to the detector. (Right, top) A top down view of the ICF target and the suspended backlight foil that sits 40 mm from the capsule. (Right, bottom) View of the ICF target near to the x-ray path that shows the 800 x 800 µm windows that are added to the hohlraum for CBI line-of-sight.

After some collaborative work with General Atomics (GA) scientist Dr. Mingsheng Wei on her HEDLP award, I accepted a staff scientist position at GA where my primary focus has become x-ray diagnostics on the National Ignition Facility (NIF). In supporting diagnostic development efforts with my NNSA-funded work, I reside full-time at Lawrence Livermore National Laboratory (LLNL) working with many experts in the field of HED science and experts in transformational diagnostics possible on the NIF scale. Having been involved in the SSAP, I had the benefit of interacting with many of these scientists prior to working at GA/LLNL, which was incredibly valuable to my development as a scientist. It also exposed me to the interests and experimental challenges that the NNSA laboratories are tackling on the frontiers of HED science and prepared me for my current work which aims to illuminate some of the unknowns in ICF capsule implosions. Presently, I am co-leading the commissioning of a quasi-monochromatic x-ray, near-normal incidence spherically-bent crystal imager called the Crystal Backlighter Imager (CBI). A cartoon of the diagnostic can be seen in Figure 1, with various views of the main ICF target and suspended backlighter foil (laser-generated x-ray source) on the right. CBI is a great diagnostic advancement as it will capture radiographs of ICF capsule implosions close to stagnation for the first time. This is possible because it has an extremely narrow bandwidth (a few eV) inherent to near-normal incidence Bragg x-ray optics that mitigates the capsule hot spot broadband self-emission which previously saturated data. This new imaging capability during the final stages of the implosion will allow the shape, integrity, and density of the shell to be measured, and it will hopefully elucidate the evolution of features, such as the fill tube and capsule support structure, that are currently not observed at these late times.

"...a total of four faculty, two research scientists, two postdoctoral researchers, 16 graduate, and six undergraduate students have been supported by NNSA programs in a little more than a decade. In 2017, five graduate students, two research scientists, and two research faculty were involved in this HEDLP research. Our graduated PhD students are working at Sandia National Laboratories, Lawrence Livermore National Laboratory, the Naval Research Laboratory, Naval Air Warfare Center, and UNR."

— A.S. Safronova, University of Nevada, Reno

National Laser Users’ Facility



Crystal Structure and Equation of State of Iron-Silicon Alloys at Earth and super-Earth Core Conditions

Princeton University ◆ PI: T. Duffy (duffy@princeton.edu) ◆ Co-Investigators: J. Wicks (Princeton), R. Smith (LLNL), and T.R. Boehly (LLE)

The metallic core at the center of a planet is important for understanding its large-scale structure, dynamics, and evolution. Unfortunately, planetary cores are difficult to study due to their remoteness and inaccessibility. The Earth's core, for example, lies below nearly 3,000 km of rock where pressures are as high as 3.6 million bars and temperatures are hotter than the surface of the Sun.

The Earth's core is composed of iron alloyed with lighter elements. The iron alloy controls phase relationships and melting temperatures in the core and may influence potential chemical reactions between the core and mantle. Silicon is a strong candidate for the core's major light element based on both cosmochemical and geochemical considerations. In addition to Earth, there is now strong interest in understanding the interior structure of large rocky exoplanets. Among the thousands of extra-solar planets discovered in recent years, those with sizes between Earth and Neptune represent the most abundant population. Experimental data are needed to understand the internal structure of these bodies.

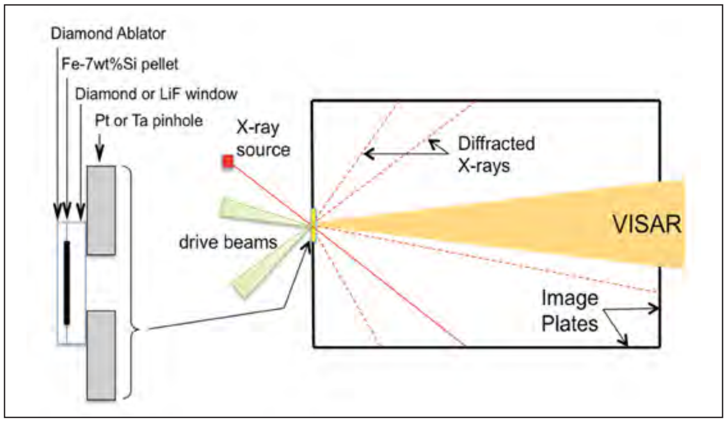


Figure 1. Schematic of dynamic ramp-compression experiments with in situ x-ray diffraction.

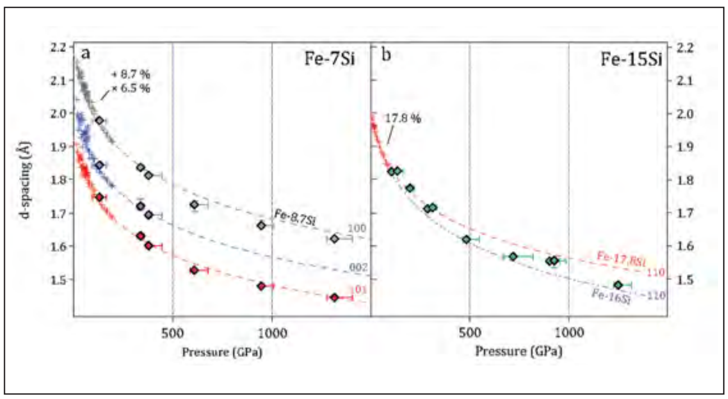


Figure 2. Measured interatomic d-spacings for iron alloys at ultrahigh pressures. The diffraction peaks for Fe-7Si correspond to the hexagonal close packed structure whereas those for Fe-15Si are for the body centered cubic structure. Low-pressure static data are shown as plus symbols and extrapolated as dashed lines.

In this NLUF-funded project, the Omega Laser was used to compress Fe-Si alloys to pressures well beyond those at the center of the Earth. Omega provides the capability to compress and probe geological and planetary materials to extreme conditions, far beyond what can be achieved with conventional static laboratory techniques. This work is part of an on-going collaboration between Princeton University, Lawrence Livermore National Laboratory, and the University of Rochester. Over the last five years, the project has provided training for three graduate students and one post-doctoral fellow.

We used the Omega and Omega EP lasers to ramp compress Fe-Si alloys reaching pressures ranging from 1.05-13.14 Mbars (see Figure 1). Iron alloyed with either 7% Si or 15% Si was used as the starting material. Our target packages consisted of a diamond/iron alloy/window sandwich. Omega laser beams were used to drive a ~10-ns ramp compression wave into the sample package. While the sample was compressed, additional beams from Omega were used to generate a quasi-monochromatic source of x-rays which then passed through the sample. X-ray diffraction peaks were recorded on image plates surrounding the sample using the PXRDIP diagnostic.

The crystal structure and equation of state of the core-forming material is its most fundamental parameter. Pure iron is expected to adopt a hexagonal-close-packed (hcp) crystal structure at the high pressures and temperatures of the Earth and super-Earth cores. Our study constrained how the presence of silicon affects the structure and equation of state. For the Fe-7Si composition, we observed 2-3 diffraction peaks that demonstrate that this alloy remains in the hcp structure to our peak pressures (see Figure 2). In contrast, the diffraction data for the Fe-15Si composition shows that it instead adopts a body-centered-cubic (bcc) structure. Thus, depending on the amount of Si in a planetary core, either the hcp or bcc structures may result. The diffraction measurements also constrain how Si affects the density of the core.

Previous models for the interior structure of exoplanets have relied on uncertain extrapolations of low-pressure experimental data. Using the new results, we constructed the first experimentally based models of large Earth-like exoplanets. Kepler—10b is a rocky extra-solar planet with a radius approximately 1.5 times that of Earth and a mass that is 3.7 times great than our planet. Using our equation of state data, we show that the incorporation of 15% silicon in this planet's iron core will increase the radius of the core by ~15% while decreasing the central pressure and density by 20% and 14%, respectively. This demonstrates that the incorporation of light elements into planetary cores may have important effects on their inferred interior structures. In future work, we will extend our efforts to constrain the properties of the silicate and oxide materials that make up the mantles of super-Earths, allowing further improvement in exoplanet interior structure models.

A Soft-X-Ray Source for Dynamic Experiments Involving Photoionized Media

University of Michigan ◆ PI: R. Paul Drake (rpdrake@umich.edu)

The National Laser Users' Facility (NLUF) project, "Experimental Astrophysics on the Omega Laser," is part of a research program led by Dr. R. Paul Drake, Dr. Carolyn Kuranz, and Dr. Paul Keiter, training students in complex hydrodynamics, radiation hydrodynamics, and magnetized flows, all of which are relevant to NNSA. During the past decade, they have graduated 14 PhDs, of which 7 have been hired into the NNSA laboratories and four are involved with NNSA projects from other laboratories, universities, or General Atomics. They now have ten doctoral graduate students, of which eight are supported in some way by NNSA funds.

Quoting the Principal Investigator, Prof. Drake, "The Omega access and other support provided by the NLUF program has enabled us to train a sequence of students in the fundamental science and experimental techniques that are used by NNSA scientists doing research on Omega, NIF, and other facilities. Our research areas—complex hydrodynamics, radiation hydrodynamics, and magnetized flows—are directly relevant to the needs of NNSA."

This research concerns dynamic phenomena, driven by photoionizing radiation, that are important to astrophysics. Phenomena of interest include photoionization fronts and irradiated clumps. Such fronts develop complex structure and were instrumental in establishing the structure of galaxies. Photoionization of clumps may or may not trigger star formation. The experiments needed a soft-x-ray source, in an open geometry, that is several ns in duration and relatively flat; previous sources of this type have been below 2 ns in duration and have not been flat.[1-3] The doctoral research of Joshua Davis has developed such a source. Two subsequent students, Robert VanDervort and Heath Lefevre, are now proceeding to use it to study irradiated clumps and photoionization fronts, respectively. This research is important for stockpile stewardship, as understanding the behavior of soft x-rays is an important topic.

Figure 1 illustrates the experiments performed to characterize the source.

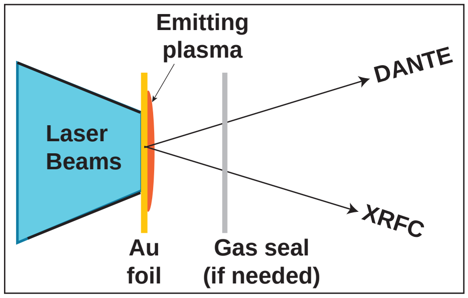


Figure 1. Schematic of experiment to measure emission characteristics of irradiated Au foil, with or without a gas seal.

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>
> — Prof. R. Paul Drake
> University of Michigan

Laser beams irradiate one surface of a thin, gold foil. Two instruments measure the emission from the rear surface of the foil. These are a multichannel spectrometer that measures the time-resolved emission (DANTE) and an x-ray framing camera that acquires images of the emission at selected times (XRFC). A separate gas seal may be included for experiments requiring high-pressure gas. In a variation on the experiment, one can irradiate the surface seen by the diagnostics to measure emission from the front side, for comparison with modeling. Both 6 ns and 4 ns pulses were evaluated.

Figure 2 shows the time dependence of the effective temperature, *T*, such that the total energy flux is given by σ*T*4, with σ being the Stefan-Boltzmann constant, for various types of gas seal as indicated. To minimize the thickness of the gas seal, and the consequent delay and reduction of *T* caused by absorption in the seal material, we mounted thin (~ 1 micron) plastic seals on metallic grids. For fixed transmission, the grids having larger openings performed better. These experiments have already produced one refereed publication,[4] with two others in preparation.

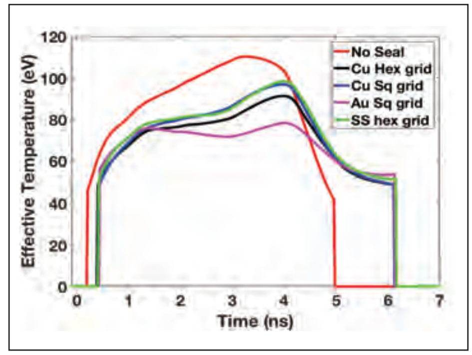

Figure 2. The time dependence of the effective temperature was affected by the gas-seal design. By comparison with no seal, the two seals using square (Sq) grids produced larger values than did those with hex (Hex) grids. The square grids had the same net transmission but smaller openings, making them more subject to hole-closure effects.

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Carlos Di Stefano, Los Alamos National Laboratory (carlosds@lanl.gov)

Years at LANL: 2015 to Present ◆ Degree: PhD, Applied Physics ◆ SSAP: 2009-2014, University of Michigan

My main role as a staff scientist in the X Theoretical Design Division at Los Alamos National Laboratory is to design and analyze high energy density (HED) experiments. The primary computational tool I use in my work is the RAGE radiation hydrodynamics code. The results from these experiments and our analysis provide valuable feedback for one of the lab's major tasks: developing computational models for hydrodynamic mixing.

During my graduate study, the support of the NLUF program was invaluable, and directly contributed to my success as an early-career scientist at Los Alamos. NLUF enabled me to do my dissertation work conducting laser-driven hydrodynamics experiments, primarily at the OMEGA laser. This experience meant that when I arrived at Los Alamos, I was able to focus immediately on learning code that I use in my design work. Further, the fact that I was already familiar with the types of experiments I would be supporting gave me a clear understanding of what I was trying to accomplish. Overall, this made the process of growing into my job efficient and effective. I also draw heavily on this background in my day-to-day work, as it helps me interpret computational results in the context of the capabilities and limitations of HED laser experiments.

One outcome of the work we are doing is the ModCons experiment,[1] short for initial modal conditions, on the OMEGA EP laser. In this experiment, we produce and diagnose HED instability growth, from repeatable initial conditions consisting of a finite multimode spectral band. An example spectrum is shown in Figure 1a. This is an interesting area of instability physics, where subgrid mixing models are not fully adequate as they ignore the specifics of the modal content, yet the behavior is more complex than can be described by single-mode analytics. Previous work[2,3] proposed the idea, and its value for testing a given model's ability to describe mode coupling. The finite band is intended to address a special problem for mode-coupling models: how to handle modes with an initial amplitude of zero.

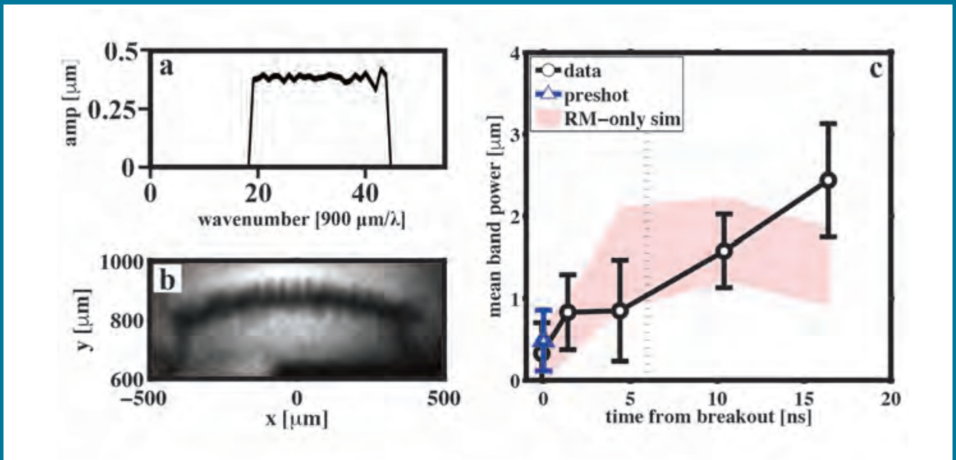

Figure 1. a) Fourier transform of the interface spectrum. Modes are seeded with uniform amplitude in a band spanning wavelengths between 20 and 47 μm, and zero amplitude elsewhere. b) An example of radiographic data. The unstable perturbation is machined at the interface between the upper edge of the dark region (denser material) and the light region above it (less dense material). c) Estimate of the mean mode amplitude within the seeded band according to our Bayesian analysis technique, both for data (open points) and a RAGE simulation (pink shaded area).

> *"During my graduate study, the support of the NLUF program was invaluable, and directly contributed to my success as an early-career scientist at Los Alamos. .... I also draw heavily on this background in my day-to-day work, as it helps me interpret computational results in the context of the capabilities and limitations of HED laser experiments."*
>
> *— Carlos Di Stefano*
> *Los Alamos National Laboratory*

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Figure 1b shows an example of the resulting data. One of the challenges of working with a modal spectrum is that it cannot be readily characterized by a single number, in the way a single-mode interface or a true broadband spectrum can. To address this, we have developed an analysis technique based on Bayesian inference (a statistical method used to update a hypothesis as more information comes in). Figure 1c shows an example of this analysis for a simple parameter, the mean band amplitude. We have demonstrated that we can use this technique to characterize other important parameters, including the analytic form of the saturated late-time spectrum and the overtaking of the seeded band by the late-time, broadband spectrum. Our current work is focused on refining the diagnostic techniques and the shape of the band to improve the robustness of our analysis.

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Students

Jacob Banasek (jtb254@cornell.edu)

Degree in Progress: PhD, Applied and Engineering Physics ◆ University/Advisor: Cornell University, Prof. David Hammer ◆ SSAP: 2014-Present

Research Topic: Thomson Scattering and Optical Spectroscopy

What are your research responsibilities?

My research has mainly focused on the development of optical diagnostic techniques for high energy density plasma experiments. One major diagnostic technique that I have worked on is using Zeeman splitting of optical lines to measure the magnetic field in a pulsed power experiment. Another major focus of my research is the development of a Thomson scattering diagnostic. This has involved finding experiments to test the capabilities of this diagnostic as well as developing code to analyze the data. The Thomson scattering diagnostic has given our lab a better understanding of the plasmas that occur within our experiments. I have also been involved in expanding the capabilities of this Thomson scattering diagnostic including setting it up to run with a streak camera, as well as the design of a multiple pulse scattering system.

How have you benefitted from the SSAP Program?

The funding provided by SSAP has given me the chance to work directly with experiments on the university scale. Having access to a machine of this scale is important as it has allowed me to have hands-on access to all phases of the experiment. This experience is valuable as it gives me a better understanding and appreciation for all phases involved in an experiment. Working on a university scale machine also allows for the freedom to try new experiential ideas, and the ability to learn from them even if they do not work.

What do you want students considering the SSAP to know?

The SSAP allows for scientific research that is important not only to stockpile stewardship but also to fundamental science to be conducted on the university scale. This allows students hand-on experience exploring important scientific questions. Being involved in the SSAP also gives access to leading scientist at the national labs, as the university scale can tackle certain problems more practically than the large national lab. This means as students we can do research that is important to the field at the university in collaboration with leaders in the field.

Paul Campbell (campbpt@mich.edu)

Degree in Progress: PhD, Applied Physics ◆ University/Advisor: University of Michigan, Prof. Karl Krushelnick ◆ SSAP: 2016-Present

Research Topic: Magnetic Reconnection Driven by High Intensity Lasers

What are your research responsibilities?

In my graduate work, I design and carry out experiments to examine magnetic reconnection driven by short pulse lasers at the OMEGA EP laser facility. A short pulse laser focused to relativistic intensities on solid targets generates strong magnetic fields. Firing two such lasers side-by-side sets up a magnetic reconnection geometry with fields strong enough that plasma conditions become relativistic. I'm working to diagnose and characterize this dynamic phenomenon with charged particle spectrometers, x-ray imaging, and proton radiography. In addition, I use particle-in-cell simulations to gain insight into the physics of magnetic field generation and the process of reconnection.

How have you benefitted from the SSAP Program?

The SSAP has afforded me the opportunity to explore magnetic reconnection at world-class facilities as a graduate student. Thanks to the National Laser Users' Facility (NLUF) program, I have conducted much of my doctoral research at the OMEGA EP laser facility at the Laboratory for Laser Energetics (LLE). In addition to my thesis work, the NLUF program trains me to perform high energy density experiments and use the diagnostic tools essential for understanding matter in these extreme conditions. With every experiment at OMEGA EP, I'm also able to expand and strengthen a network of collaborators and colleagues at LLE, the national labs, and industry partners. SSAP support has also allowed me to travel to conferences and workshops to present my work and expand my understanding of the field.

Have you spent time at one of the national laboratories?

Before starting at the University of Michigan, I spent a summer as an undergraduate intern at Lawrence Livermore National Laboratory with a team of scientists, postdocs, and students at the Jupiter Laser Facility. There, I was introduced to ultrafast lasers, nonlinear optics, plasma physics, and high energy density science. I attended lectures and National Ignition Facility group meetings and was exposed to a scientific community outside of my university.

This experience was invaluable in shaping my academic path. I was inspired to pursue a PhD studying high intensity laser-plasma interactions at the University of Michigan. I hope to have the opportunity to return to the national lab setting and continue collaborations initiated by the NLUF support.

Rachel Flanagan (rflanaga@eng.ucsd.edu)

Degree in Progress: PhD, Mechanical Engineering ◆ University/Advisor: University of California, San Diego, Prof. Marc Meyers ◆ SSAP: 2016-Present

Research Topic:Investigation of Material Behaviors Under Extreme Conditions Though Nonequilibrium Simulations

What are your research responsibilities?

I perform nonequilibrium molecular dynamics simulations of materials in extreme environments. My thesis research is focused on the response of materials such as silicon carbide and irradiated copper undergoing shock deformation at pressures of 5-150 GPa. This work is motivated by experiments performed at various NNSA laboratories, where my colleagues conduct gas gun and laser ablation experiments to generate shock waves. Molecular dynamics simulations allow us to investigate the atomic mechanisms behind phase changes, spallation, and other shock-related phenomenon by tracing and visualizing the motion of individual atoms. Together, our experiments and simulations work to validate and explicate material behaviors in extreme environments.

How have you benefitted from the SSAP?

The SSAP provides a strong intellectual environment for my work. To accurately model the systems we are interested in requires computational models with several billions of atoms - such simulations are typically cost-prohibitive. The SSAP has supported collaborations with Los Alamos National Laboratory where the use of high performance computing resources has enabled such massive simulations to run in a modest amount of time. Finally, the SSAP also provides opportunities for me to connect with other scientists with similar interests by funding my conference trips and summer research. Over the past summer, I visited Los Alamos National Laboratory, where I collaborated with experimentalists and other theorists to develop models that more accurately characterize the behavior of irradiated materials. This collaboration offers me the chance to continue developing my skillset as a computationalist while I progress towards my doctoral degree.

Did the SSAP influence your choice of research area and university?

My father is a United States Marine, and his commitment to service and country has always inspired me to hone my skills towards supporting my country in some capacity. From my early teens, I was passionate about science so rather than joining the military, I thought it would be best to pursue what I was most talented at. As an undergraduate, I was drawn to both physics and mechanical engineering, allowing me to develop a highly unique, interdisciplinary skill set. Upon learning about the SSAP, the interdisciplinary nature of its mission, and the opportunities available through the program, I knew that the SSAP would allow me to begin pursuing a highly fulfilling career in scientific research.

Rebecca Lewis (lewis@nscl.msu.edu)

Degree in Progress: PhD, Nuclear Chemistry ◆ University/Advisor: Michigan State University, Sean Liddick ◆ SSAP: 2016-Present

Research Topic: Indirect Neutron Capture Cross Sections for Nuclear Astrophysics

What are your research responsibilities?

I am part of a collaboration working on determining the neutron-capture cross sections of short-lived nuclei involved in the r-process (i.e. the rapid neutron capture process) using indirect methods. Direct measurement of these cross sections is not feasible due to the short half-lives of the nuclei involved, so instead I use the beta decay (i.e. radioactive decay in which an energetic electron or positron and a neutrino are emitted) of nearby nuclei to obtain statistical information about the nucleus formed in neutron capture. This information can be used to calculate a neutron capture cross section. This process, known as the β-Oslo method, allows us to reduce the uncertainty in neutron capture cross sections for very neutron-rich nuclei. I am involved in the planning, setup, execution, and analysis of experiments using this method. The experimental techniques translate easily to other experimental programs and I'm able to assist many other experiments at the National Superconducting Cyclotron Laboratory (NSCL) that utilize similar detectors and analysis.

How have you benefitted from the SSAP?

I have been able to interact with many different people in nuclear science that I otherwise might never have met. The ability to step back and see the full breadth of the research being done, especially in national security, is very exciting. I have been exposed to a significant quantity of forefront research that is different but complementary to what I do, and was different from what I even thought was available in nuclear science. The experience has allowed me to think about what kind of science I want to pursue in the future.

Have you spent time at one of the national laboratories?

My funding from the SSAP allowed me to spend three months at Los Alamos National Laboratory working on a project for my thesis that I would not have been able to accomplish by myself at the NSCL. I worked with staff scientists who actually wrote some of the complicated statistical reaction model code that I was using for my project, which allowed me to leave LANL with completed, publishable work. The daily interaction with knowledgeable experts at the national laboratory accelerated my progress on my project and my thesis as a whole.

Cecilia Eiroa Lledo (cecilia.eiroalledo@wsu.edu)

Degree in Progress: PhD, Chemistry ◆ University/Advisor: Washington State University, Prof. Nathalie Wall ◆ SSAP: 2015-Present

Research Topic: Thermodynamic Properties of Technetium(IV) in Halide Containing Systems

What are your research responsibilities?

My main research responsibility is to determine thermodynamic parameters of Tc(IV)-halide complexes, with the final goal of observing the dependence of Tc(IV) solubility with halide concentration in aqueous media. The rationale for this work is that the determination of Tc(IV) solubility in presence of halide will aid the understanding of the mobility of Tc(IV) in environmental systems. To determine the thermodynamic parameters for Tc(IV) with the halides, I use several techniques. Liquid-liquid extractions (LLE) experiments are performed to determine the Gibbs Free energy of reaction; radiochemical analyses of Tc(IV) are conducted using liquid scintillation counting. The enthalpy (equals the internal energy plus pressure times volume) and entropy (which measures disorder of a system) of the systems are derived using the van't Hoff analysis (which explores changes in EoS functions) in which the Gibbs free energy of the solution is determined at different temperatures. The solubility of Tc(IV) in halide containing systems will be determined experimentally through solubility studies, and theoretically by the application of the thermodynamic parameters found through LLE.

How have you benefitted from the SSAP?

Being part of the SSAP has allowed me to develop my technical skills and understanding of basic nuclear sciences. Through this program I was able to become a nuclear reactor operator at Washington State University's 1 MW TRIGA reactor. Having a reactor license has given me the chance to learn about reactor theory, basic nuclear chemistry and technical knowledge for the handling of radioactive materials. In addition, I am able to produce my own Tc-99m samples at the reactor, and use it as material for my research. The skills that I have learned thanks to this program have helped me become a better scientist with a better understanding of basic knowledge needed in the field of radiochemistry and nuclear science.

What do you want students considering the SSAP to know?

Being part of the SSAP will give you many opportunities for growth in technical and basic knowledge in your area of interest. The skills you will develop under this program will help you reach your career goals by exposing you to intellectually challenging projects, and by interacting with scientists that will serve as mentors throughout your research. The experiences you gain through this program will further your understanding of the fields of nuclear sciences, and give you a chance to reach out to national laboratories, or to pursue projects you never thought you would.

Zachary Matheson (matheson@nscl.msu.edu)

Degree in Progress: PhD, Nuclear Physics ◆ University/Advisor: Michigan State University, Prof. Witold Nazarewicz ◆ SSAP: 2015-Present

Research Topic: Theory of Nuclear Fission

What are your research responsibilities?

I carry out advanced calculations to predict the fission properties of heavy nuclei, such as fission half-lives and yield distributions. The primary goal of my thesis is to improve the workflow for performing fission calculations using an existing nuclear density functional theory (DFT) solver, and then to use it to study various nuclei, such as superheavy nuclei for astrophysical r-process research or actinides for reactor research. The nucleus I am currently studying is Oganesson-294, a superheavy element which was discovered jointly by scientists from Dubna (Russia) and Lawrence Livermore National Laboratory (LLNL), and is currently the heaviest element ever produced by humans. I am also trying to extend the current model to describe slow-neutron induced fission.

How have you benefitted from the SSAP?

While working on my thesis, the SSAP has allowed me to engage in projects that are both relevant and intellectually satisfying. Furthermore, by working with the SSAP and the NNSA, I have been granted access to work on some of the most powerful computing systems in the world. Apart from making my research possible, this means that I have gained experience working in some of the world's most advanced high-performance computing environments, with some of the greatest support and resources available. Finally, I have been invited to participate in SSAP events, which has made me aware of career opportunities available to people in, or related to, my field of research.

Have you spent time at one of the national laboratories?

I spent six months working at LLNL with the lead developer of the DFT solver I use in my research. Through this I was also able to participate in the development of new features and extensions to the code, and I gained a lot of insight into the theoretical model, its strengths, and its limitations.

In fact, one of the primary benefits to me of being at LLNL and collaborating with a variety of nuclear/programmatic scientists was that I began to see my research in the context of a greater whole. I could see the importance of what I am working on now, and I also gained exposure to other areas of research in the lab where my training may lead to useful contributions in the future.

Emil Petkov (emilp@unr.edu)

Degree in Progress: PhD, Physics ◆ University/Advisor: University of Nevada, Reno/Dr. Alla Safronova ◆ SSAP: 2012-Present

Research Topic: Applications of X-ray Spectroscopy and Spectropolarimetry to HEDL Plasmas

What are your research responsibilities?

My research as a graduate student at the University of Nevada, Reno primarily consists of the study and analysis of radiation from high-energy-density laboratory (HEDL) plasmas. This involves a combination of spectroscopic imaging analysis, signals processing, and non-local thermodynamic equilibrium (non-LTE) modeling of experimental data. I also focus on studying the atomic physics of highly ionized ions by using plasma polarization spectroscopy. This diagnostic relies on both atomic physics of highly charged ions and general plasma physics knowledge, and is a very important and novel tool for studying HEDL plasmas. Recently, I have been involved in the study of x-ray line polarization of multiply ionized Mo ions produced on the Lawrence Livermore National Laboratory (LLNL) electron beam ion trap. The results were used to benchmark predictions of theoretical codes, which can then be applied to study HEDL plasmas. In the past 5 years, I have disseminated my work at various conferences while also writing papers for peer-reviewed journals.

How have you benefitted from the SSAP?

The benefits provided by the SSAP program are truly invaluable. Along with providing financial support for my graduate studies, it has allowed for me to travel to a variety of meetings, including the yearly SSAP symposium, and engage with other professionals in the high-energy-density plasma physics community. The meetings and interactions have enriched my general understanding and opened my eyes to a multitude of research areas that lie within my field. The SSAP has also allowed me to develop great relationships with collaborating researchers, and to learn more about their areas of study. For example, I learned a lot from scientists at LLNL while working with them last year on the LLNL electron beam ion trap. This lent a great deal of insight into how to effectively engage in collaborative efforts with resident staff at a national laboratory.

What do you want students considering the SSAP to know?

The SSAP provides a tremendous benefit to the students that it supports. On the surface, the funding is very helpful in aiding in the opportunity to travel to conferences and the yearly SSAP symposiums. On a deeper level, you get to network and meet professionals in your field and related fields. The relationships you develop with fellow colleagues at universities, as well as scientists from national laboratories, will be of substantial value for your career.

Alexander Ramus (arasmus@umich.edu)

Degree in Progress: PhD, Applied Physics ◆ University/Advisor: University of Michigan, Dr. Carolyn Kuranz ◆ SSAP: 2012-Present

Research Topic: Coupled Hydrodynamic Instabilities on Oblique Interfaces

What are your research responsibilities?

I primarily perform experiments studying hydrodynamic instabilities driven by shocks on the Omega EP laser. I design targets, specify the laser and diagnostic configuration for the experiments, and analyze the resulting data. I work in tandem with a designer who performs radiation-hydrodynamics simulations of the experiments. Hydrodynamic instabilities on interfaces are of critical importance to the performance of inertial confinement fusion (ICF) implosions, mixing cold, higher Z material into the central hot-spot. When a shock is incident on a perturbed interface, vorticity is deposited due to misaligned pressure and density gradients. The subsequent evolution of the interface is called the Richtmyer-Meshkov (RM) process. When the incident shock is tilted relative to the mean interface, a bulk shear flow is also driven across the interface, resulting in a Kelvin-Helmholtz (KH) instability component to mixing width growth. Low-mode asymmetries in ICF implosions lead to non-parallel shocks and interfaces, implying that in addition to RM growth, there is a KH growth component due to the shock acceleration of interfaces. In order to study this coupled instability growth, I perform experiments at Omega EP in which a sustained shock is launched across a perturbed, tilted interface.

How have you benefitted from the SSAP?

SSAP has provided funding for my research and travel throughout my PhD through continued support of the Center for Laser Experimental Astrophysics Research, allowing me to do a variety of research at Stanford Linear Accelerator Laboratory, Los Alamos National Laboratory (LANL), Lawrence Livermore National Laboratory, and the Univerity of Rochester Laboratory for Laser Energetics. During experiments at LANL, funded in part by the SSAP, I met a LANL scientist who I now work for while finishing my PhD. I've been in residence at LANL for nearly half of my PhD, and working at the lab has afforded me access to experimental facilities, scientific expertise, and computational support that have made my thesis work possible. Two scientists at the lab who perform simulation and design work for my experiments, Carlos Di Stefano and Forrest Doss, were also supported by SSAP while graduate students at the University of Michigan. My time at LANL has given me exposure to a broad range of high energy density (HED) and ICF research, helping me better understand how my research fits into HED community as a whole. I'm pursuing post-doctoral positions at the national laboratories as I reach the end of my PhD, and SSAP has given me both the research experience and connections to make that possible.

Robert VanDervort (dervort@umich.edu)

Degree in Progress: PhD, Applied Physics ◆ University/Advisor: University of Michigan, Prof. R. Paul Drake ◆ SSAP: 2014-Present

Research Topic: Experiments to Understand the Interaction of Stellar Radiation with Molecular Clouds

What are your research responsibilities?

My thesis project is to design an experimental platform to explore radiation transport regimes. The platform should enable the study of transport regimes between the optically thick and thin limits, by changing the density of a target foam. The foam sphere is driven by x-ray radiation from a laser-irradiated, thin, gold foil. Measuring the response of the sphere, such as changes in density profile, over this range will provide data useful to understanding how to better apply radiation transport in simulations. As a primary investigator for this experiment, I am responsible for designing, executing, and analyzing the resultant data for future experiments. My most important responsibility is effectively communicating the experimental results to collaborators and the community at large. Communicating with both experimental and simulation collaborators is essential to enable successful experiments.

How have you benefitted from the SSAP?

The SSAP has provided opportunities to attend and contribute to many exciting and diverse experiments. The SSAP has provided the opportunity to learn the tools necessary to assist experiments on Janus at the Jupiter Laser Facility and conduct experiments at Omega. Presentation opportunities are frequently available. I have presented research at numerous conferences including posters at Omega Laser User Group, NIF User Group, and presentations at the American Phyiscal Society Division of Plasma Physics. The SSAP has provided the ability to gain breadth in the field of laboratory astrophysics.

Have you spent time at one of the national laboratories?

I spent the summer of 2015 as a graduate-student intern at Los Alamos National Laboratory. Through this internship, I was able to explore topics that as an experimentalist I would not otherwise study. I learned how to setup simulations to resemble an experiment. I learned how to use simulations to inform experimental data and provide design parameters for future experiments. During my internship, I compared self-emission data from University of Michigan experiments on Omega 60 to xRage simulations of a similar target. The internship gave me the opportunity to meet with experts in laboratory astrophysics. The presentation of research was encouraged. I presented in both an oral and poster format. As a result of this internship, I now have a better understanding of what working at the laboratory is like. I am excited to pursue a career at a national laboratory.

Bryan Zuanetti (bxz135@case.edu)

Degree in Progress: PhD, Mechanical and Aerospace Engineering ◆ University/Advisor: Case Western Reserve University, Dr. Vikas Prakash

SSAP: 2014-Present ◆ Research Topic: Dynamic Resistance of Metals Under Extreme Conditions

What are your research responsibilities?

My research is focused toward achieving a better understanding of underlying mechanism(s) that control the in-elastic response of metals under thermomechanical extremes, especially at strain-rates beyond 10^4/s. At low loading rates, flow stress of metals is understood to be controlled by a thermally-activated mechanism in which the interaction between dislocations and short-range barriers provides the largest contribution towards the flow stress. In this strain-rate regime, there is good agreement between models and experimental findings. However, at higher loading rates (beyond ~5,000/s) experimental findings suggest a shift in the dominant mechanism(s) which controls the dislocation motion. The resultant dynamic material behavior is difficult to probe experimentally, especially at elevated temperatures; consequently, in the past few years, I have worked on the development of novel test procedures and laser-based diagnostics associated with the extension of a conventional single-stage gas gun to elevated temperature to probe the dynamic mechanical response of metals under extreme conditions.

How have you benefitted from the SSAP?

The SSAP has been the primary source of funding for this research at Case Western Reserve University. The SSAP funding has enabled us to pursue our research interests and develop the tools necessary to attempt to answer some of the important scientific questions posed in our research. Additionally, it was through the SSAP annual meetings that I had the chance to meet with well-established scientists in the shock compression physics area, which led to opportunities for summer internships and collaborations with the national labs.

Have you spent time at one of the national laboratories?

I spent the summer of 2017 at Los Alamos National Laboratory (LANL). While at LANL, I had the opportunity to perform experiments where an ultrafast laser was used to generate supported shock waves through thin metallic films pre-heated to the desired test temperatures. By studying the decay of the resultant stress waves through different thickness samples, the rate sensitivity of the sample materials was investigated at ultra-high loading rates. These experiments have been beneficial to my thesis since they have enabled me to probe the dynamic behavior of metals, of interest to my work, at loading rates unachievable in our current plate impact facility at Case. Besides new experimental capabilities, my stay at LANL provided me the opportunity to interact with experts in my field in a casual setting, which has provided valuable insights to several experimental and computational aspects of my work relevant to my research project.

Predictive Science Academic Alliance Program II

STANFORD UNIVERSITY

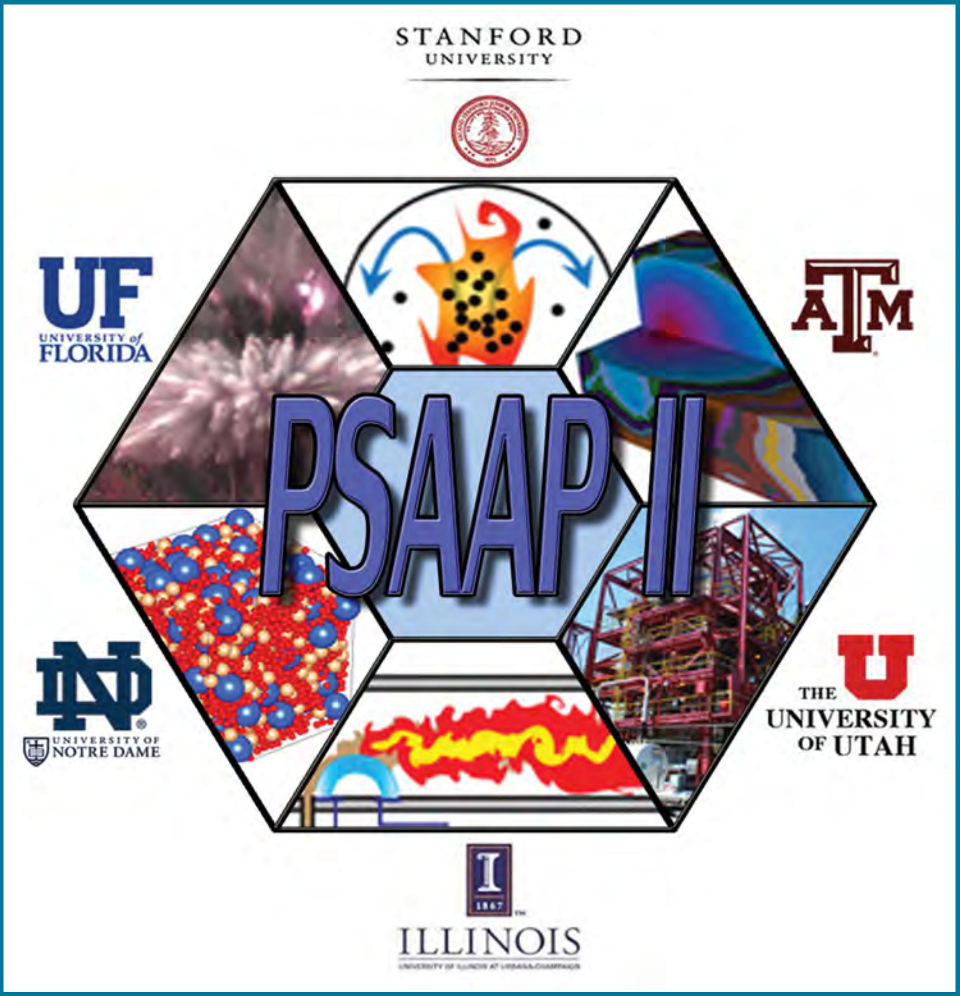
ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

THE UNIVERSITY OF UTAH

UF
UNIVERSITY of FLORIDA

Predictive Science Academic Alliance Program II
Overview

Predictive Science Academic Alliance Program (PSAAP) II is a five-year program established in 2014 by the Advanced Simulation and Computing (ASC) program of the National Nuclear Security Administration to demonstrate predictive science in an extreme-scale computing environment. Each of the following centers is using a multi-scale and multiphysics application as a focus for their research, and is applying state-of-the-art verification and validation techniques in order to undertake predictive science with uncertainty quantification. Three of the sites are Multidisciplinary Simulation Centers (MSCs) and three are Single-Discipline Centers (SDCs) funded at approximately $4 million and $2 million, respectively.



- University of Florida, “Center for Compressible Multiphase Turbulence”
- University of Illinois-Urbana-Champaign, “Center for Exascale Simulation of Plasma-Coupled Combustion”
- University of Notre Dame, “Center for Shock Wave-processing of Advanced Reactive Materials”
- Stanford University, “Predictive Simulations of Particle-laden Turbulence in a Radiation Environment”
- Texas A&M University, “Center for Exascale Radiation Transport”
- University of Utah, “The Carbon-Capture Multidisciplinary Simulation Center”

Due to the complexity of the applications, predictive science can only be done on the most powerful computers available. Thus, the intent is to develop and demonstrate technologies and methodologies to support effective extreme computing leading to exascale by focusing on these science and engineering applications. Each center is utilizing a different computing environment to support the simulation of their application and provide the necessary data for validation and uncertainty quantification. These simulations are being performed on a variety of systems made available by the ASC at the NNSA national laboratories and by the Office of Science at Argonne National Laboratory and Oak Ridge National Laboratory.

One of the unique characteristics of the program is that every student supported with PSAAP II funds must spend an internship of at least 10 weeks at one of the NNSA national laboratories. The program is in its fourth year and, to date, over 100 students have taken advantage of the opportunity. These internships provide the laboratories with access to students who are exposed to the complexity of conducting research on multi-disciplinary problems in a high performance computing environment. This exposure has led to the hiring of over 20 students following completion of their PhD degrees.

Each of the six Centers is briefly discussed on the following pages.

Predictive Simulations of Particle-laden Turbulence in a Radiation Environment

Stanford University ◆ PI: Gianluca Iaccarino (jops@stanford.edu)

The PSAAP II research project at Stanford University aims at advancing the state of the art in large-scale predictive simulations of irradiated particle-laden turbulent flow to improve energy harvesting in Concentrated Solar Power (CSP) systems. To this end, a flexible and efficient High-Performance-Computing (HPC) framework suitable for Exascale supercomputers is being developed. The figure corresponds to an instantaneous snapshot post-processed from a Point-Particle Direct Numerical Simulation of the volumetric particle-based solar receiver designed within the project. The setup consists of a turbulent gas-particle mixture advected through a square duct, with dimensions 7W x W x W (W = 4 cm), and volumetrically irradiated in the transverse direction. The objective is to maximize the transfer of energy to the fluid by means of micron-size particles that absorb and convect the incident radiation to the gas phase. The bulk Reynolds number of the flow is Re = 20000, the particle-size distribution is approximated by 5 different classes with Kolmogorov Stokes numbers, i.e., ratio between particle and fluid relaxation times, in the range $5 < St < 20$ and with a total mass fraction ratio of MFR = 40%. The test section is radiated from one side on a 4W x W area with a power of P = 3 kW. Similar to the experiment, a development section is utilized as a turbulent particle-laden generator that provides inflow conditions for the radiated section. To properly capture all the significant flow scales (integral to Kolmogorov), the simulation requires a resolution of 55M cells per section, the particles are approximated by 30M Lagrangian points per section, and the transport of radiation energy is characterized by means of a Discrete Ordinates Method (DOM) with 7M cells and 350 quadrature points. The figure depicts a zoomed-in visualization of the radiated region; particle-laden turbulent flow in the streamwise direction from left to right, incident radiation in the y-axis direction from below. A slice on the streamwise x-y plane has been extracted to facilitate the visual access to the inner part of the duct. The quantity represented is temperature (ranging from 300 to 430 K) of the gas and particles. A temperature iso-contour (T = 400 K) is also shown to illustrate the direction of the incident radiation. It is interesting to note (1) the presence of elongated particle clusters resulting from preferential concentration, i.e., phenomena by which inertial particles tend to avoid intense vorticity regions and accumulate in regions of high strain rate; (2) the accumulation of particles at the walls as a result of turbophoretic effects, i.e., tendency of particles to migrate towards regions of decreasing turbulence levels; (3) the absorption of radiation by particles and the corresponding exponential decay in the perpendicular direction; and (4) the transfer of thermal energy from the particles to the fluid and the subsequent thermal mixing enhanced by turbulence. The software development and numerical simulations have been performed on NNSA systems and on Titan and Mira supercomputers of the Oak Ridge (OLCF) and Argonne (ALCF) Leadership Computing Facilities.

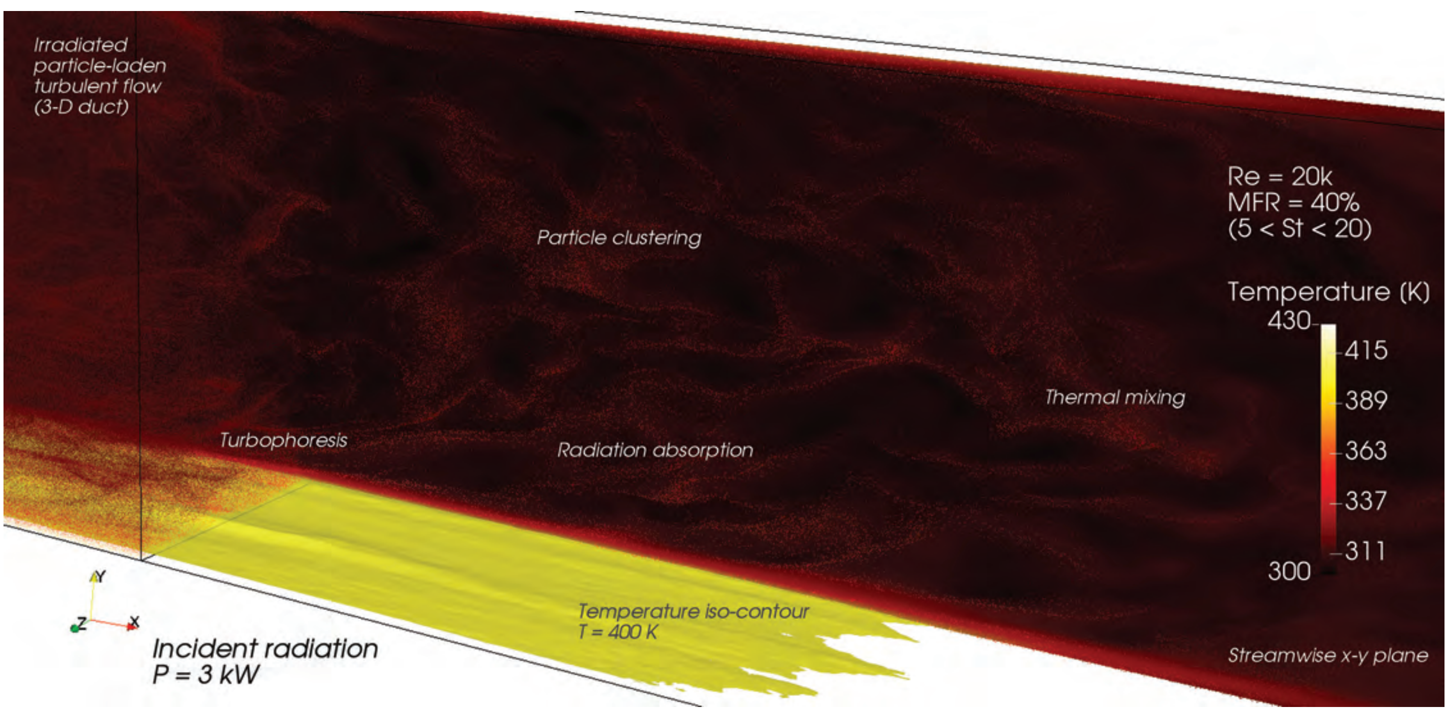


Figure 1. A zoomed-in visualization of the radiated region; particle-laden turbulent flow in the streamwise direction from left to right, incident radiation in the y-axis direction from below.

Texas A&M University ◆ PI: Jim Morel (morel@tamu.edu)

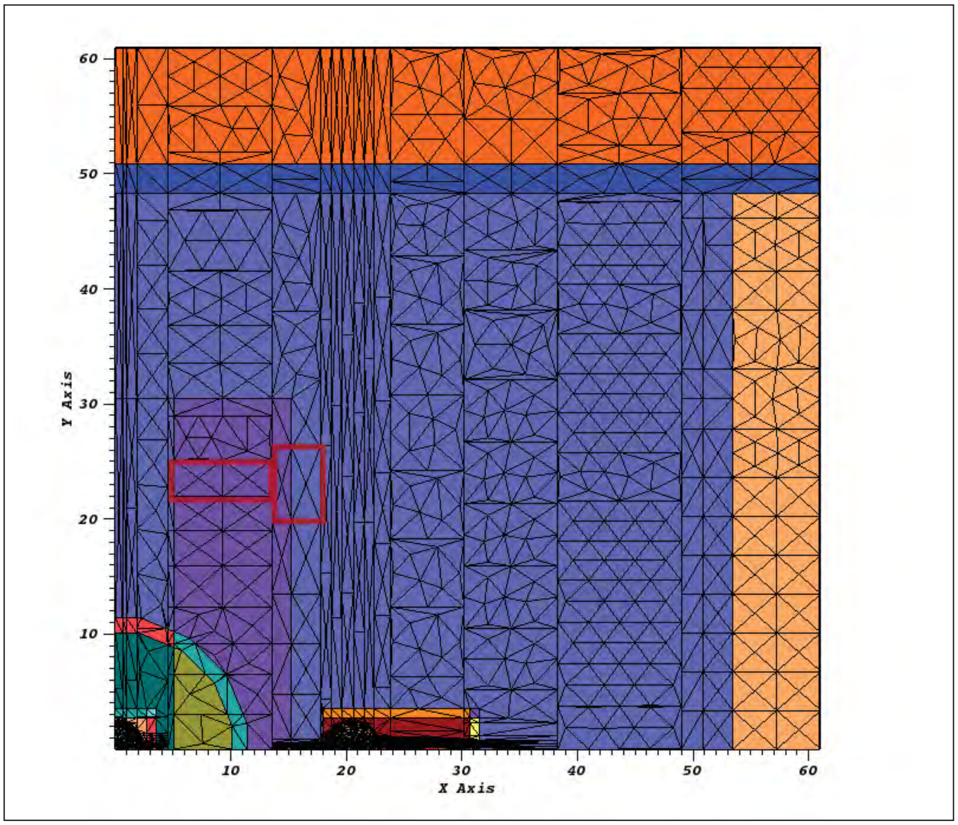


Figure 1. 2D cut-plane view of 3D mesh generated using the adaptive mesh refinement-type macro mesh generation method. Two macro mesh cells (processor domains) are outlined in red.

The Center for Exascale Radiation Transport (CERT) research is focused on radiation transport and includes development of transport methods for exascale computing. Exascale computing refers to computing systems capable of at least a billion billion calculations per second. CERT is developing the following: algorithms for propagation of thermal radiation through high-temperature matter in the high energy density physics (HEDP) regime; general-purpose exascale computer-science algorithms; numerical methods and subgrid models for radiation propagation; methods for quantifying prediction uncertainties; and experiments that test computational predictions and associated uncertainty quantification.

Perhaps the most significant accomplishment of this year was the development of special unstructured mesh generation techniques and associated load-balancing algorithms for thermal radiation transport calculations. Standard massively-parallel transport solution techniques rely on processor domains corresponding to non-reentrant subsets of the spatial mesh. A processor domain is a portion of the mesh assigned to a processor which will perform all the computation associated with that domain. A non-reentrant domain has a physical shape such that radiation passing through that domain along any straight line enters and leaves that volume only once. Re-entrant domains degrade the efficiency of the standard solution process. Achieving non-reentrant processor domains is easy to achieve on rectangular meshes, but it is essentially impossible on standard unstructured meshes. To achieve this, we first impose a uniform rectangular macro mesh over a complex geometry. Each macro cell in the mesh is non-reentrant since it has the form of a rectangular box. Each processor then builds an independent unstructured mesh for its non-reentrant domain. Next a global conformal mesh is obtained by "stitching" the processor domains together, i.e., by adding mesh vertices on the processor domain boundaries to eliminate any hanging vertices. Such vertices occur when a cell face is shared by more than two cells. Eliminating hanging vertices requires a capability for polyhedral mesh cells since a cell can end up with an arbitrary number of faces. If the mesh contains very different length scales, the number of cells may vary widely between processor domains causing a load imbalance in that different amounts of computational work will be required for different processors. Such imbalances are inefficient. The smallest total computation time is achieved with an equal load for each processor. Our first improved procedure for load balancing was to generate a non-uniform rectangular macro mesh after generating a uniform macro mesh with the goal of keeping the number of unstitched cells in each macro mesh cell as constant as possible. Once the final macro-mesh has been defined, remeshing within each macro cell is done, followed by stitching. Our second improved procedure was to replace a non-uniform rectangular macro grid with an adaptive orthogonal macro grid that allows macro cell faces to be shared by more than two macro cells. The increased flexibility of such a grid enables us to better meet the goal of a constant number of cells within each processor domain. A full spatial grid generated with an adaptive macro grid is illustrated in Figure 1. More specifically, this graphic represents a two-dimensional (2D) cut through a 3D mesh. Two macro grid cells are outlined in red. For this grid we were able to reduce the ratio of the largest number of cells per processor domain to the average number of cells per processor domain to 1.76. With the non-uniform rectangular macro mesh method, the ratio was 2.63, and with the uniform macro-mesh method, the ratio was 41.82. Thus the load balance was improved by over a factor of 20 with our latest method. Further improvements should lead to ratios very close to one. Earlier this year, we sponsored a grid-generation workshop attended by staff from the DOE/NNSA national laboratories. It was very well received highlighting the fact that the highest levels of parallel transport efficiency can only be obtained on unstructured grids through the use of special grid-generation techniques.

The Carbon Capture Multidisciplinary Simulation Center (CCMSC)

The University of Utah ◆ PI: Philip J. Smith (philip.smith@utah.edu)

The Carbon Capture Multidisciplinary Simulation Center (CCMSC) is partnered with General Electric (GE) to develop predictive, science-based, digital representations of full-scale options for increasing efficiency and minimizing carbon footprints on worldwide projects delivering electric power from coal. The Center has a goal of using near-exascale computational power to predict new radical boiler concepts with accuracies of 5% in the quantities of interest to the power generation designers. This objective requires the tightly-integrated efforts of the three equally funded CCMSC sub-teams: the computer science team, the physics team, and the validation/ uncertainty quantification (V/UQ) team. The uncertainties in model forms, operating scenarios, computational numerics, and experimental data are captured and propagated to the overarching prediction. The evidence for achieving 5% uncertainties in a prediction of some potential future facility relies on a hierarchical validation composed of experimental data from carefully selected facilities. This V/UQ computational effort requires not only simultaneous consistency between all the experimental data in the hierarchy but also ensures that the sensitivities of the overarching quantities of interest are reflected in the experimental data obtained in the smaller-scale devices where the data are available.

The CCMSC predictive design of a 0.5 gigawatt electric (GW_e) power plant has evolved from a 5,000 m^3 design to a 50 m^3 system by exploiting supercritical CO_2 (sCO_2) Brayton power cycles with carbon capture. By using a pressurized, entrained-flow, oxy-coal gasifier operating at 25 bar, it appears possible to not only reduce the physical size of the device, but to also double power efficiencies while obtaining a near zero carbon footprint. The gasifier delivers the option of using either an open or closed Brayton cycle. Figure 1 represents a large eddy simulation of one instantiation of the design of this gasifier. The image was produced using volume-rendering tools developed by the Center and integrated into VisIt, the Lawrence Livermore National Laboratory visualization software.

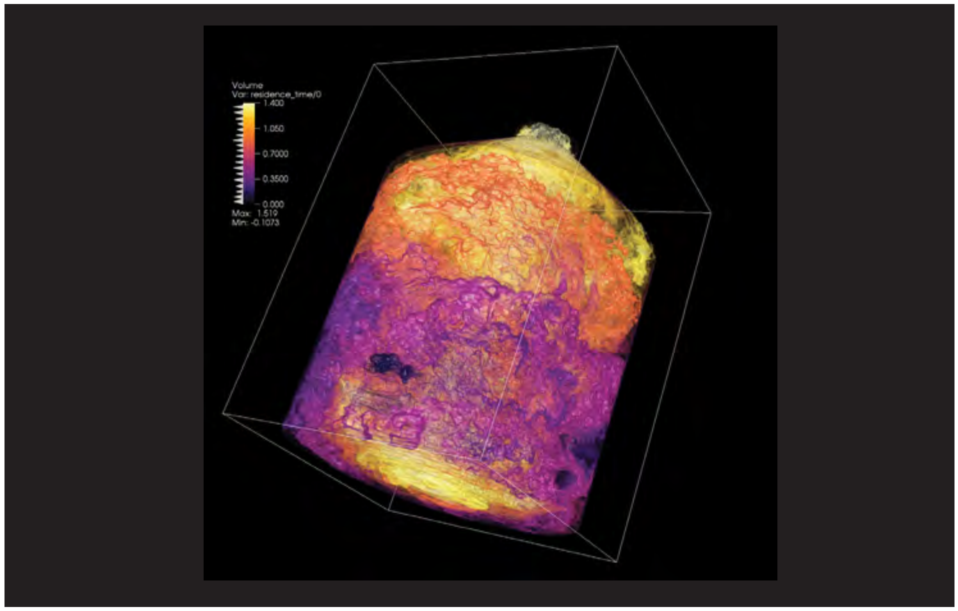


Figure 1. A volume rendered image of the residence time distribution in the high pressure oxy-coal gasifier design.

The simulation demonstrates the value of the Uintah runtime developed by the Center for delivering scalability up to 256,000 processors for a fully integrated multi-physics problem with particle and gas transport and reaction, coupled with radiative, convective, and conductive heat transfer. These computations were performed on LLNL's Vulcan and Argonne National Laboratory's Mira using an INCITE award.

In order to accomplish the goals of the CCMSC, this project leverages existing computational resources, but is also aimed at running efficiently at exascale. CCMSC has adopted the Sandia National Laboratories Kokkos project to provide performance and portability on next-generation heterogeneous hardware. Paired with the Uintah MPI and task based parallelism, Kokkos offers data parallelism with minimal demands for reformatting on the underlying physics code. Significant research is also focused on managing data for these extremely large computational scales, both from an I/O and visualization perspective using the CCMSC's PiDX project.

The faculty, staff, and students working on this project are delivering: 1) exascale-ready computing software that is regularly released through open-source licensing, 2) tools for V/UQ for use with other large applications with expensive function evaluations and sparse/expensive experimental data, and 3) new advances in computer science, software engineering, computational fluid dynamics, multiphase reacting flow, and radiative heat transfer.

Center for Compressible Multiphase Turbulence

University of Florida, Gainevsville ◆ PI: S. Balachandar (bala1s@ufl.edu) ◆ Technical Manager: Thomas L. Jackson (tlj@ufl.edu)

The overarching goals of the Center for Compressed Multiphase Turbulence (CCMT) are threefold: (1) to radically advance the field of compressible multiphase turbulence (CMT) through rigorous first-principle multi-scale modeling; (2) to advance very large-scale predictive simulation science on present and near-future platforms; and (3) to advance a co-design strategy that combines exascale emulation with a novel energy-constrained numerical approach. The Center is performing petascale, and working towards exascale, simulations of instabilities, turbulence, and mixing in particle-laden flows under conditions of extreme pressure and temperature.

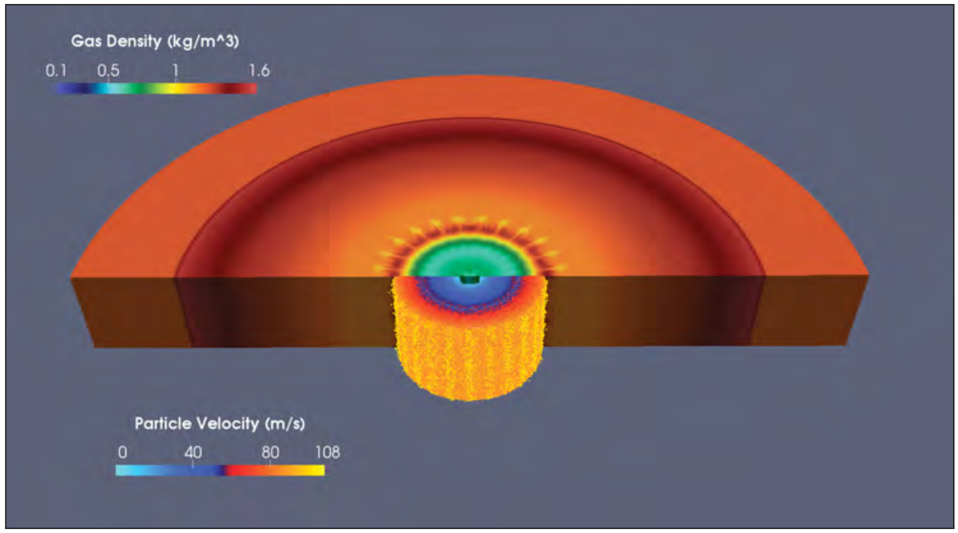


Figure 1. Multiphase three-dimensional simulation of cylindrical blast wave; time 1.25 ms.

The overarching demonstration problem consists of a cylindrical core of explosive surrounded by an annular region of polydisperse metal particles. The shape and amount of the explosive charge and the size distribution of the metal powder and its material are parameters that are varied. Simulations of the demonstration problem were successfully carried out on the DOE supercomputers Quartz and Vulcan, and a number of prediction metrics were compared to experiments; see Figure 1 for a typical simulation output. The state-of-the-art simulations of this problem at the micro (O(1000) particles), meso (O(10^9) particles) and macroscales, along with validation-quality experiments, allow us to better understand the fundamental physics of compressible multiphase turbulence and translate this understanding to modeling and simulation of a wide variety of problems of national importance. For example, at the microscale, recent three-dimensional simulations of shock propagation through a random bed of particles has led to the development of next generation pairwise extended point-particle force models that systematically incorporate effect of nearest neighbors. Uncertainty reduction is a key goal of the center and it drives micro and mesoscale-informed model development, apart from error reduction in both experimental and numerical approaches. Simulation and experimental uncertainty budgets determine the biggest contributors to the overall uncertainty and the drive to reduce these biggest uncertainties dictate the Center's focus.

An important development of the co-design process is the emergence of CMT-nek as a powerful higher-order spectral discontinuous-Galerkin compressible multiphase flow code which combines finite element and finite volume ideas to solve the governing equation and scales to million cores. Figure 2 shows results from mesoscale simulation of an expansion fan moving through a bed of particles and regions of large volume fraction variation can be observed in the volume rendered image. Since the particles that are initially sequestered at the bottom of the tube expand over time to occupy a much larger volume, a dynamic load balancing algorithm has been developed to obtain about a factor of 8 speed up in some applications. Another unique contribution of the Center is the use of field-programmable gate arrays for exascale behavioral emulation of the performance of CMT-nek on future exascale architectures. We have developed behavioral emulation (BE) methods and tools to support algorithmic design-space exploration (DSE) of key CMT-nek algorithms on notional future architectures and systems. The key kernels and communication patterns of CMT-nek are abstracted into a mini-app (CMT-bone) and modeled as application BE Objects (BEOs). Similarly, existing systems and architectures are modeled as architecture BEOs. These models are calibrated and validated through benchmarking. Validated models are then extended to represent notional systems to support algorithmic DSE.

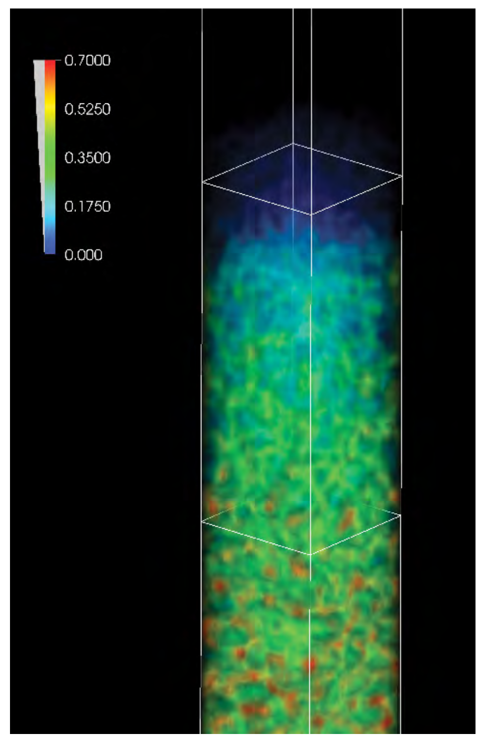


Figure 2. Multiphase three-dimensional simulation of an expansion fan moving through a bed of particles.

The Center for Exascale Simulation of Plasma-Coupled Combustion (XPACC)

University of Illinois at Urbana-Champaign ◆ PI: William Gropp (wgropp@illinois.edu)

The Center for Exascale Simulation of Plasma-Coupled Combustion (XPACC) has an overarching mission to advance the science and technology of plasmas to initiate and control turbulent combustion. This mission drives research efforts in both multi-physics predictive simulation and the computer science techniques to harness the exascale-class computational platforms necessary for high-fidelity simulations.

The figure shows an example of the 300 “full-scale” simulations conducted recently to map the ignition threshold for a round hydrogen fuel jet exhausting into a turbulent air crossflow. The ignition is mediated by a co-annular dielectric-barrier discharge plasma actuator and seeded by the optical breakdown of a focused laser. Multiple simulations were used to add value to the prediction by mapping the threshold, determine sensitivity to uncertain model parameters fundamental to the three-dimensional configuration (e.g., the scale-resolved turbulent trip), and assess the impact of uncertain model parameters on the uncertainty of the predicted quantity of interest. These full-scale simulations were the final stage of a series of low-dimensional (0D, 1D and 2D) physics-targeted configurations designed to identify pacing uncertainties and calibrate models for the physical sub-mechanisms, including chemical kinetics, plasma kinetics, and optical breakdown. Insensitivity to resolution of the turbulence scales was established in conjunction with a weak scaling study with up to 4x the resolution of the baseline full resolution simulations. These were conducted primarily on Quartz and Vulcan at LLNL, as well as on Titan at ORNL to evaluate dependence on these different hardware platforms. The largest of these had ~2.5 billion mesh points.

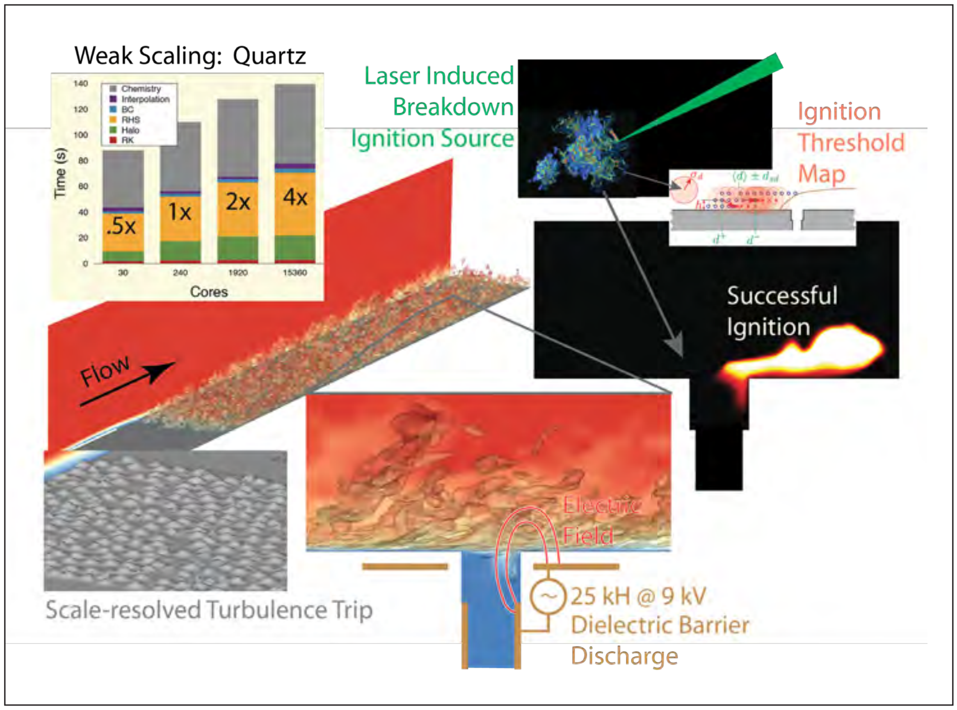


Figure 1. Sustained ignition threshold mapping of a hydrogen fuel exhausting into a turbulent boundary layer.

The principal simulation tool PlasComCM/2 used high-order finite-difference methods on three overset structured meshes. The short time scales of the laser-induced breakdown made it relatively straightforward to simulate its early stages in a separate specialized radiation transport equation solver coupled with flow equations. The dielectric barrier discharge required only a single coupled electric field solve, employing a plasma kinetics model that was studied in detail in an axisymmetric geometry with corresponding experiments and advanced diagnostics, some of which were conducted at Sandia National Laboratories.

The simulations were run with the ICE (Illinois Coding Environment) annotation system, which allows a user to direct the compiler to (also optionally) invoke alternate hand-optimized code, undertake autotuning, and target routines for just-in-time (JIT) recompilation at runtime, taking into account the runtime parameter values. It carries negligible overhead, and in some examples showed significant speed-up, with the JIT tool Moya finding vectorization opportunities that were unavailable at the initial compilation. These and planned capabilities are realized with the same source code designed by the computational scientist, which compiles naturally on nearly every system (MPI, Fortran, C/C++). ICE is designed to invoke additional performance tools, from XPACC or other efforts. Additional tools for hardware flexibility and performance are being designed and invoked by ICE for future simulations.

University of Notre Dame ◆ PI: Karel Matouš (kmatous@nd.edu)

The Center for Shock Wave-processing of Advanced Reactive Materials (C-SWARM) is dedicated to developing predictive computational tools for multiscale modeling of heterogeneous materials under extreme conditions that will execute effectively on future Exascale platforms. Through adaptive simulations, C-SWARM's goals are to predict conditions for the synthesis of novel materials and provide prognoses of non-equilibrium structures that will form under shock wave-processing. Using this approach, researchers at C-SWARM plan to identify conditions under which they can synthesize cubic boron nitride (c-BN). They will then duplicate the conditions in the laboratory in order to demonstrate the effectiveness of their predicted conditions. c-BN has many applications since its hardness is similar to that of diamond, but its thermal and chemical stability is superior.

C-SWARM scientists employ adaptive multiscale and multi-time computational schemes to model reactive powder materials that are used during shock wave-processing. Moreover, the C-SWARM team is developing novel numerical techniques such as the adaptive wavelet method, and the parallel generalized finite element solver (PGFem3D). Students and research staff benefit greatly from working on a difficult problem that requires an interdisciplinary approach involving teams of researchers in conjunction with high-performance computing.

The modeling of high-energy reactive materials requires complex constitutive equations. The computational physics team has proposed a new continuum theory for powders that couples pressure sensitivity and rate dependence of cold compacted materials, and has performed large parallel thermo-mechanical simulations on NNSA computing platforms (see Figure 1). After detailed calibration, verification, and validation, such complex simulations are used for design and analysis of computer experiments. In particular, the computational physics team performs predictive simulations and optimizes the design conditions to increase the pressure, density, and temperature conditions during gas gun experiments.

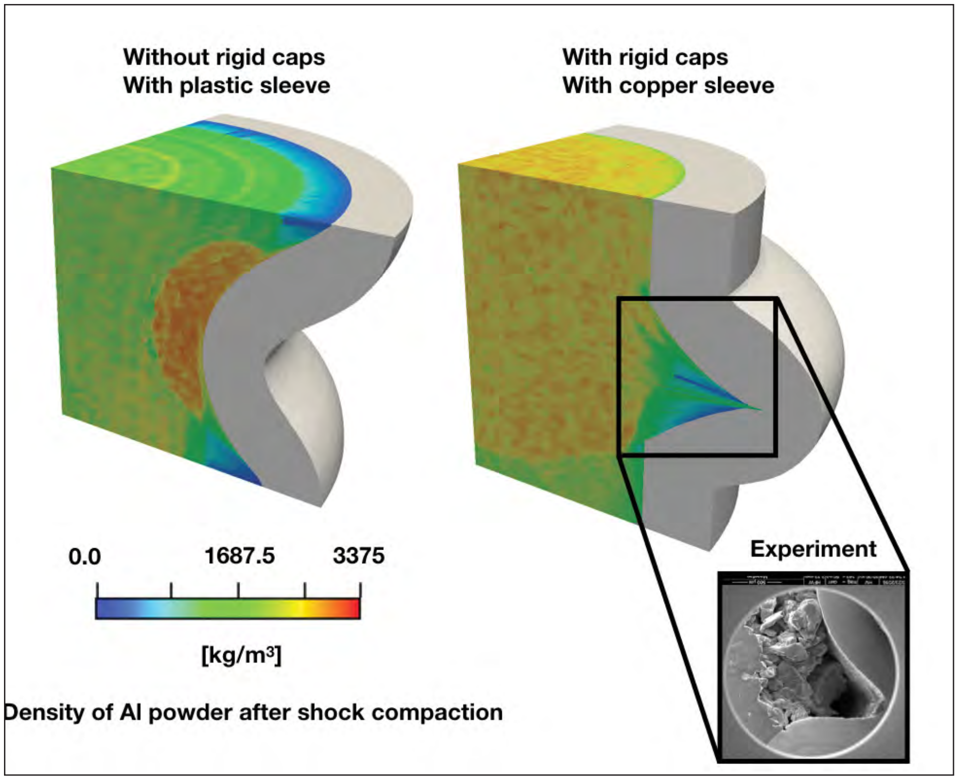


Figure 1. Simulations using a new continuum theory for powders with comparison to experimental data.

Based on the computational design, the experiments are performed to confirm the validity of the predictions. Once fully completed, C-SWARM's collaborative and interdisciplinary framework can be the basis for Virtual Materials Testing standards and aid in the development of new material formulations.

An advanced asynchronous multi-tasking runtime system and advanced software libraries support the C-SWARM software applications. The modular implementation of the multi-tasking runtime system (HPX-Lite) enables both performance and productivity. Moreover, to separate scientific applications from details of the runtime system, C-SWARM researchers are developing a Domain Specific Embedded Language and Active System Libraries that are based on the concepts of generic and meta-programming techniques to effectively eliminate the penalty that frequently arises from abstractions. The researchers from the computer science team are focusing on the development of Matrix and Tensor Template Libraries (MTL/TTL), Photon networking, multiscale graph scheduling, adaptive wavelet multi-processing, and Exascale architectures.

The integrated V&V/UQ program provides a platform for verification, validation, and propagation of uncertainties. The emphasis of C-SWARM is on quantifying the predictive ability of the multiscale simulations in an efficient manner. The key component is a series of carefully co-designed experiments and data-driven simulations (with quantified uncertainties) to enable meaningful and rigorous comparisons of simulation predictions with experimental results.

Stewardship Science Graduate Fellowship

Matthew R. Gomez, Sandia National Laboratories (mrgomez@sandia.gov)

Years at Sandia: 2011 to Present ◆ Degree: PhD, Nuclear Engineering and Radiological Sciences ◆ SSGF Program: 2007-2011, University of Michigan, Dr. Ronald M. Gilgenbach

I am presently a principal investigator for inertial confinement fusion experiments on the Z machine at Sandia National Laboratories, New Mexico. Our fusion experiments are called Magnetized Liner Inertial Fusion. In these experiments we fill a pencil-eraser-sized metal cylinder or "liner" with an isotope of hydrogen called deuterium, which is capable of undergoing nuclear fusion. An axial magnetic field of 10 Tesla is applied to the fuel, and a terawatt laser beam is used to heat the fuel to a few million Kelvin over several nanoseconds. An 80-terawatt electrical pulse is passed through the metal cylinder causing it to implode until it stagnates which squeezes both the preheated fuel and the axial magnetic field. The axial magnetic field prevents the fuel from losing all of its energy to the cooler metal walls during the implosion, and as a result, the fuel temperature rises dramatically to nearly 30 million Kelvin through adiabatic compression. At the temperatures and densities produced in these experiments, the deuterium fuses, releasing energy and producing neutrons.

The experiments that I am conducting are focused on understanding the conditions produced at stagnation such as temperature, density, and plasma volume/shape for a given set of input parameters. Working with a team of computational experts as well as other experimentalists, we use what we learn to design new experiments with increased stagnation performance. This requires developing new diagnostics and analysis techniques. An example of one such diagnostic is our high-resolution continuum x-ray imager, which measures monochromatic x-rays emitted by the hot deuterium plasma. An image obtained with this diagnostic is shown in Figure 1. Data collected with the diagnostic have provided evidence of instability feedthrough in our high convergence stagnation column, which has helped direct our focus towards experiments with higher initial fuel density and lower expected convergence.

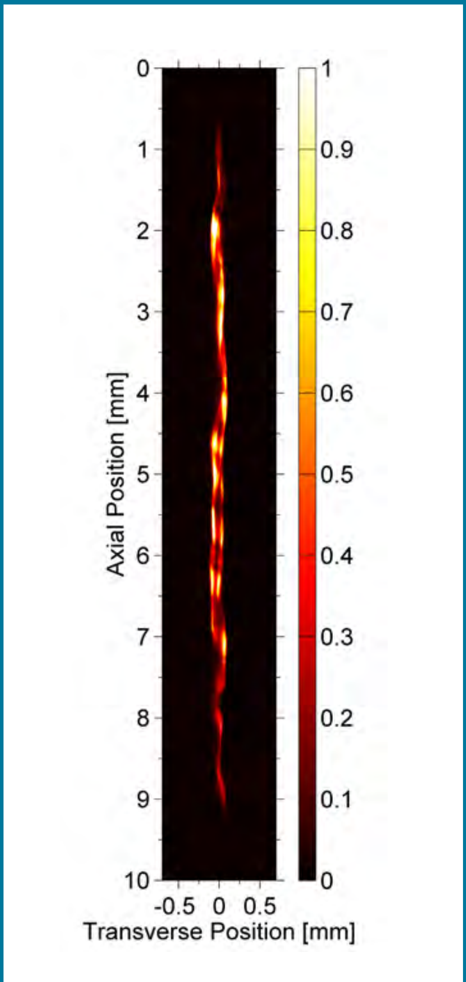


Figure 1. X-ray self-emission image of the stagnation column in Magnetized Liner Inertial Fusion. The variations in signal intensity come from a combination of variations in fuel conditions and differences in the x-ray opacity of the surrounding liner material.

Before I came to Sandia full time, I conducted my graduate research at the University of Michigan with Professor Ronald Gilgenbach as my advisor. I was in the second class of Stewardship Science Graduate Fellows, and as a part of the program I completed a practicum at Sandia. This was my first direct exposure to the Z Machine and the high-energy-density physics experiments that it was designed to drive. The focus of my practicum was to set up a visible spectroscopy system for use on the Z Machine. I used the system to study plasma formation in the transmission lines that deliver the electrical pulse from the driver to the target. Fielding this diagnostic on a variety of experimental campaigns allowed me to interact with many scientists and managers. These connections were extremely helpful in finding a position after graduation. I ended up being hired by the same manager that I worked under during my practicum. I owe a lot to the Stewardship Science Graduate Fellowship program, and as a result I have tried to remain involved in the program to help out the new classes of fellows.

"I conducted my graduate research at the University of Michigan with Professor Ronald Gilgenbach as my advisor. I was in the second class of Stewardship Science Graduate Fellows, and as a part of the program I completed a practicum at Sandia. This was my first direct exposure to the Z Machine and the high energy density physics experiments that it was designed to drive."

— Matthew R. Gomez
Sandia National Laboratories

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Charles Epstein, cepstein@mit.edu

Degree in Progress: PhD, Physics ◆ University/Advisor: Massachusetts Institute of Technology, Prof. Richard Milner ◆ SSGF: 2014-Present

Research Topic: Radiation in Electron-Electron Collisions

What are your research responsibilities?

I work on an experiment that aims to measure radiative Møller scattering: the process in which two electrons collide and (sometimes) emit a photon. Our current understanding of this is insufficient for a variety of new, precision low-energy experiments. In particular, most calculations have neglected the electron mass, which has significant effects at low energies. As a graduate student, I've worked on updating the theoretical calculations, writing code to simulate collisions, and on designing and running a new experiment to validate the theory. We're currently commissioning the experiment at the Massachusetts Institute of Technology High Voltage Research Laboratory.

How have you benefitted from the SSGF Program?

The SSGF program has, aside from the excellent financial support, allowed me to broaden my knowledge of stewardship science. During my practicum at Lawrence Livermore National Laboratory (LLNL), I was able to learn about a new field of research in Planetary Defense which I would never have otherwise had the opportunity to experience. I really enjoyed the national lab atmosphere, and am grateful to have been introduced to that career path option. I also have had the opportunity to meet and connect with a wonderful group of peers, both at LLNL and at the SSGF Annual Program Review.

Did the SSGF Program give you the opportunity to work with others you might not have otherwise?

Through the SSGF Program, I was able to spend my practicum working at LLNL with Paul Miller and Tane Remington in the field of Planetary Defense. Their group studies the threat of asteroid impacts with Earth, and the possible ways to mitigate the hazard. Some of these mitigation methods include either a kinetic impactor, or a nuclear device. We worked on hydrodynamic simulations of rock collisions, and on tuning them to match data. These simulations are useful for understanding the outcome of colliding an asteroid with a device intended to push it off course. I focused on examining the effects of parameters that describe the flaws along which the rock will fracture. The simulations and computational methods were very different from those I had previously experienced. Being able to learn a new scientific perspective, in an exciting and different research environment, was an extremely valuable experience. If not for the SSGF, I would not have had the chance to take part in this work.

Nathan Finney, nrfinney@gmail.com

Degree in Progress: PhD, Mechanical Engineering ◆ University/Advisor: Columbia Unversity, Dr. James Hone ◆ SSGF: 2015-Present

Research Topic: Two-Dimensional Materials Under Extreme Conditions

What are your research responsibilities?

I am building crystallographically aligned boron-nitride/graphene/boron-nitride systems to study the physics of strongly commensurate single-crystal layered composites. To do so I am mechanically rotating these layered materials relative to one another by pushing on them with an atomic force microscope, and verifying alignment with friction feedback and Raman spectroscopy measurements. Currently we are studying the electronic structure of these hybrid systems at low temperature and high magnetic field. Once we thoroughly understand the electronic structure of these aligned systems, we plan to apply extreme strain & pressure to observe how their electronic and mechanical properties evolve under extreme conditions.

How have you benefitted from the SSGF Program?

The lab practicum and annual SSGF program reviews provide an opportunity to visit the impressive facilities at DOE/NNSA labs, as well as an opportunity to learn from laboratory scientists who support our stewardship science mission. Also, the freedom to focus on research has proved to be invaluable.

What do you want students considering the SSGF to know?

As a developing researcher, your main contribution at this stage is your own intellectual development. You are learning how to be a scientist! The SSGF is incredibly supportive in this regard by providing you with opportunities to meet and work with professional laboratory scientists who support the stewardship science mission. There are many opportunities for mentorship in this program.

Did the SSGF Program influence your choice of research area and university?

The SSGF program motivates me to focus on materials that exhibit interesting properties under extreme conditions (strain, temperature, magnetic field, etc.), which aligns quite well with my choice of university and research group.

How has this been beneficial to your research? Your future career?

Doing the lab practicum after the first year of my program was a perfect primer for research. The practicum was kind of like a mini-PhD, or "Nano-PhD" as my practicum advisor Dr. Worsley jokingly referred to it. My advisor and one of his postdocs provided focused guidance, which allowed me to learn new fabrication procedures, and conduct measurements using tools and materials I had not used before. I had to conduct extensive literature reviews to get my bearing in an area of research outside of my comfort zone (material synthesis and characterization, specifically for graphene aerogels). Group meetings provided opportunities for feedback, always constructively critical and kind. By the end of the summer I was able to confidently present my work at the summer student poster session.

Cole Holcomb, cholcomb@astro.princeton.edu

Degree in Progress: PhD, Astropysical Sciences ◆ University/Advisor: Princeton University, Prof. Anatoly Spitkovsky ◆ SSGF: 2014-Present

Research Topic: Nonlinear Cosmic Ray Transport

What are your research responsibilities?

Cosmic rays are charged particles traveling at near-light speeds through the interstellar and intergalactic media. Despite their small number densities, the cosmic ray kinetic energy makes up a substantial fraction of the total energy in the Milky Way. This abundance of free energy allows these atomic scale particles to influence galactic scale structures. For example, they have recently been implicated in producing galactic winds that evacuate interstellar gas from the galactic disk, arresting the formation of new stars.

My role is to investigate the kinetic physics of cosmic ray transport through interstellar space. I use the electromagnetic Particle-in-Cell numerical method to calculate the motions of tens of millions of energetic particles as they stream along magnetic field lines threading the interstellar plasma. The goal is to excite fluctuations in the magnetic field (Alfvén waves) that are thought to be unstable in the presence of these streaming cosmic rays. The rates at which these waves grow and the amplitudes that they attain ultimately determine how strongly the cosmic rays can drive galactic scale change. These simulations will inform macrophysical fluid simulations and enhance our understanding of how galaxies and galaxy clusters evolve.

How have you benefitted from the SSGF Program?

Having a funding source external to my university has opened up a myriad of opportunities, both in my research and my personal life. The stipend has allowed me to keep teaching assistant and grading responsibilities to a minimum and to really focus on my research, which has been instrumental in finishing my projects to my satisfaction in the five year limit of my doctoral program. The SSGF meant that I never worried that a lack of funding would prevent me from following the research path I truly wanted. I am continually grateful for the support that the SSGF has provided.

What do you want students considering the SSGF to know?

I honestly look forward to the yearly Program Review. The talks and activities have been eye-opening experiences in which I've learned about subjects I would otherwise almost certainly never have come into contact with. The SSGF is full of great people that I've enjoyed getting to know over the years. On top of that, we have a lot of fun together. I've always come away from the review feeling refreshed and invigorated.

Brooklyn Noble, brooklyn.noble@utah.edu

Degree in Progress: PhD, Mechanical Engineering ◆ University/Advisor: University of Utah, Prof. Bart Raeymaekers ◆ SSGF: 2015-Present

Research Topic: Nanotribology and Lubrication Fundamentals

What are your research responsibilities?

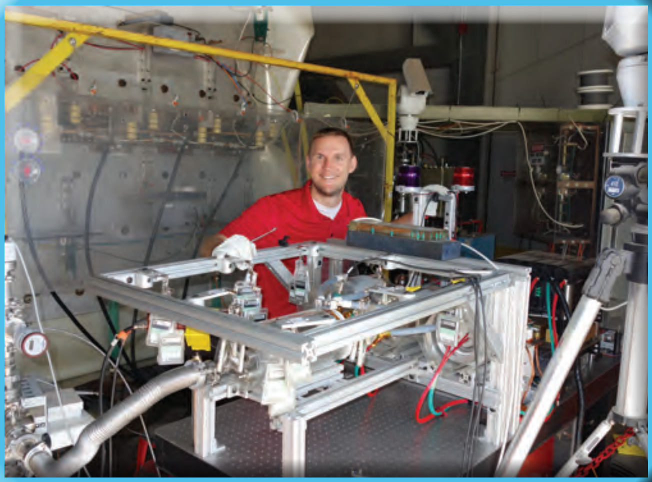
My research responsibilities include working with parallel computer code and interfacing with supercomputers to solve Newton's equations for systems of thousands of atoms in order to simulate their trajectories one femtosecond at a time. With these simulations, I am working to understand physical phenomena that were observed in experiments. I try to obtain a nanoscale understanding and link to macroscale observations in order to create design-guidelines for applications that use ultrathin lubricant systems. With this understanding comes the ability to address the challenges that currently limit the effectiveness of ultrathin films used in a variety of engineering applications such as: micro- and nanoelectromechanical devices, nanoimprint lithography, antibiofouling coatings which remove or prevent microorganisms on wetted surfaces, and hard disk drives, which are ubiquitous in consumer electronics, medical devices, and industries such as microfabrication, food processing, and marine shipping, among many others.

How have you benefitted from the SSGF Program?

The SSGF program allowed me to be very efficient with my graduate school experience. During the academic year, I was able to gain depth of knowledge and fully focus on my doctoral research because the fellowship ensured I would not need to worry about other funding opportunities like teaching assistantships. During the summer, I was able to gain breadth of knowledge and explore a research opportunity at a national laboratory with a different scope than my doctoral research, an opportunity I might not have had otherwise. I got to experience what a career at a national laboratory would be like and create a network that will be very valuable when I am ready to begin my career.

What do you want students considering the SSGF to know?

Students considering the SSGF should know that this fellowship is truly remarkable. To be the recipient of any fellowship is a great honor. However, the SSGF is a step above in the opportunities it creates for its fellows. Because of this fellowship, I have had the opportunity to tour multiple laboratories and scientific historic sites around the country, engage with fellows from widely varying research fields, and even perform research at a national laboratory. The network created between fellows, alumni, and top scientists is unparalleled. With full tuition benefit, research allowance, a competitive stipend, an engaging annual meeting, opportunities to experience national laboratories, and a great network of support, this fellowship creates the ideal graduate research experience.



Feature Articles

An Overview of LLNL's Physics Internship Program

Britton Olson, Computational Physicist and High Energy Density Physics Student Coordinator (olson45@llnl.gov), Lawrence Livermore National Laboratory

Introduction

The High Energy Density Physics (HEDP) Summer Student program brings in the most qualified and talented graduate and undergraduate students to work on a diverse collection of research projects. HEDP students are amongst the hundreds that join Lawrence Livermore National Laboratory's (LLNL's) ranks each summer to conduct research and take advantage of the rich scientific community it offers. Students in the program spend three to four months working side-by-side and one-on-one with their project mentors to pursue novel research with high impact potential. This program is an excellent opportunity for beginning graduate students in the SSAP to establish connections at LLNL for future residency and employment.

Mira's Magnets

Mira Partha

Sharing a name with a red giant star in the constellation Cetus, Mira Partha has always dreamed of understanding the fiery reaction that keeps stars burning— nuclear fusion. A student at the Massachusetts Institute of Technology (MIT), Partha has spent the last three years pursuing her passion for fusion energy, first at MIT's Plasma Science and Fusion Center, and now at Lawrence Livermore National Laboratory. She shares this vision of an energy source that is clean, efficient, and effectively unlimited with scientists around the world who are working on harnessing the power of nuclear fusion, the same process that powers the sun.

The fusion of deuterium and tritium is known to produce large amounts of energy. Getting deuterium and tritium to fuse, however, is no small feat. Scientists at the National Ignition Facility (NIF) attempt to achieve this via a method called indirect drive inertial confinement fusion (ICF). In this process, energy from 192 laser beams is deposited on the walls of a gold hohlraum that contains a tiny capsule, roughly 1 mm in diameter. This capsule encloses layers of deuterium-tritium (D-T) ice and D-T vapor which act as the fusion fuel. The hohlraum walls absorb the energy carried by the laser beams, and emit radiation that bathes the capsule. The material from the capsule's outer surface ablates off and the fuel is compressed inwards—similar to a spherical rocket. As the fuel compresses, the fuel may ignite, generating large quantities of energy through D-T fusion reactions. Minor asymmetries in the capsule and laser drive produce hydrodynamic instabilities that greatly diminish energy output. Studying the effects of these asymmetries (see Figure 1) is the first step towards mitigating energy loss enough such that a break-even point on yield can be achieved.

That's where Mira Partha's work comes in. Under the mentorship of Steven Haan, Partha has spent the last two summers utilizing the high-performance computing infrastructure at LLNL to perform simulations examining the effects of the magnetic fields generated during asymmetrical implosions, via a phenomenon called the Biermann Battery. The Biermann Battery is a process by which weak magnetic fields are generated from zero initial conditions. Previous work on the subject suggested that these self-generated magnetic fields would have a beneficial impact, via increases in thermal conductivity. However, no comprehensive studies had been done to quantify these effects.

Using new capabilities in the multi-physics code HYDRA, Partha has surveyed a broad array of implosion configurations, including many that are commonly encountered in NIF experiments. She examined impact on yield metrics such as number of neutrons produced, or average ion temperature, to find the implosion geometries that display the most significant effects of self-generated magnetic fields. With nearly two terabytes of data produced

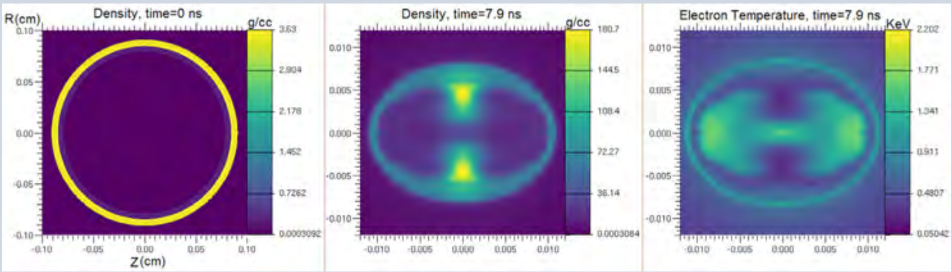


Figure 1. Shows simulations of an imploding ICF capsule perturbed by an early-time asymmetry in the radiation drive. Left shows the initial density of the capsule. Center and right show density and electron temperature, respectively, of the imploded capsule at late time. The large scale asymmetries which have formed will reduce the fusion yield of the implosion.

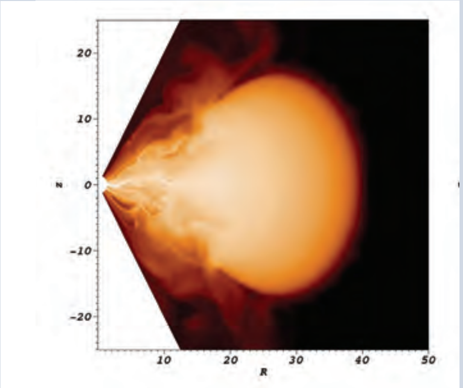


Figure 2. The mass density of a magnetized black hole accretion torus simulation of Cosmos++. The black hole is the white circle at the left. Magnetic fields stimulate the magneto-rotational instability in the torus which seeds turbulence, dissipates angular momentum, and triggers accretion flow streams that eventually hit the black hole giving rise to x-ray emissions and jet ejecta.

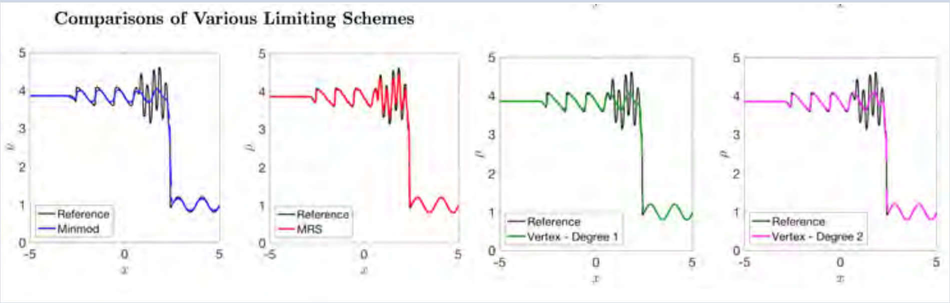


Figure 3. Results from various limiter schemes on the 1D Shu-Osher test problem. This problem demonstrates the limiter's ability to discern between the physical oscillations (left of the shock or density jump) and small numerical oscillations caused by the shock itself. All the schemes are effective in damping out the numerical oscillations. However, the method of Moe, Rossmanith, and Seal (MRS) [2015, arXiv:1507.03024] was designed for DG methods and resolves the oscillations to the left of the shock and is in better agreement with the reference solution (black) than the other methods tested.

thus far, Partha has studied the impact of the Biermann battery in several distinct geometries, for a wide range of perturbation amplitudes. She has documented that the Biermann battery has an impact ranging from 2-20% on the fusion yield. She has also examined in detail the physical mechanisms underlying these effects—changes in thermal conductivity, instability growth, and alpha particle transport, among others. Additionally, her work has aided in code validation for various inchoate features in HYDRA, enabling more accurate simulations for future work.

Partha's work is part of an important effort to accurately account for current discrepancies between physical experiments and simulations. Improved computational models enable optimized experiment design that maximizes energy return, bringing us one step closer to achieving this ideal energy source. As Partha would say, once we conquer nuclear fusion, the stars will be within our reach.

Colton's Code

Colton Bryant

Colton Bryant grew up pursuing passions of skiing, raft guiding, and kayaking. On a whim, while attending Colorado School of Mines, Bryant took a class that changed the course of his life, Linear Algebra. Since then Bryant has shifted his focus to pursuing a career in research in the field of applied mathematics. Bryant is currently a PhD student in Engineering Sciences and Applied Mathematics at Northwestern University where he works on the development of numerical methods for studying particles confined to fluid interfaces.

Though Bryant's research interests began in a classroom, he has learned that they have astronomical implications. Bryant's mentor, LLNL Physicist Peter Anninos, has explored galaxies and the physics that govern their formation and destruction. Peter uses a simulation code named Cosmos++ and LLNL's massive supercomputers to run simulations of complex astrophysical phenomena. Black hole accretion disks, for example (see Figure 2), form as the mass from a star or other body is pulled into a spiraling orbit into a black hole. The dynamics of how this occurs literally determines how stars are born or die. These events are impossible to recreate in experiments on earth, too complex for theory, and too far away to observe directly.

The lessons learned from these calculations are only as good as their accuracy. This is where Bryant's work comes in. For the past two summers Bryant has worked as an intern in the HEDP program at LLNL studying ways to make Cosmos++ more accurate.

Discontinuous Galerkin (DG) finite element methods allow for arbitrarily high order approximations to gradients inside each computational cell without increasing the amount of communication between processors on the supercomputer. The finite element method is a numerical method which subdivides a large problem into smaller simpler parts called finite elements, or cells. DG combines features of the finite element and the finite volume frameworks. However, there are some drawbacks to DG: small oscillations in the solution are introduced near steep features, such as a shock wave, in a simulation. These unphysical oscillations can grow and eventually cause the accuracy to be lost. The techniques Bryant has been investigating are called slope limiters, which work by tracking the oscillations at each time step and adding the necessary smoothing or dissipation to damp out non-physical waves. The fundamental question is how to use the limiters without sacrificing accuracy near physical extrema and real oscillations.

Bryant's work has involved implementing and testing several of these limiting techniques to identify the pros and cons of each type of method for various situations. The results have been promising, and slope limiters have allowed for high order accuracy to be used even in problems where shocks are present (see Figure 3). The limiters are able to adjust the solution near these sharp features while recognizing and turning off near physical oscillations.

The slope limiters studied by Bryant are a key feature in improving the accuracy of Cosmos++ and will give Anninos and his collaborators greater confidence in the real world astrophysical problems they explore.

How to Apply

The call for applications for the HEDP Summer Student Program opens in the Fall with applications due early February. The online application can be found at https://scholars.llnl.gov and searching for "high energy density intern."

Postdoctoral Fellows

Dana M. Dattelbaum, Program Manager (danadat@lanl.gov) and Thomas Nizolek, Postdoctoral Fellow, Los Alamos National Laboratory

Postdoctoral fellows are an integral and crucial partner in the success of the NNSA national laboratories, tackling the research and development challenges associated with NNSA-related mission science. At any time, Los Alamos National Laboratory (LANL) has approximately 400 postdoctoral fellows working across a diverse set of organizational divisions, scientific disciplines, and National capabilities. A postdoctoral opportunity at the Laboratories offers unprecedented access to some of the Nation's unique experimental and computational platforms. Within the Dynamic Materials Properties experimental portfolio at Los Alamos, for example, postdocs are leading research using x-rays from U.S. Light Sources at the Advanced Photon Source (APS) and at the Linac Coherent Light Source (LCLS), including the newly-commissioned Dynamic Compression Sector and High Pressure Collaborative Access Team beamlines at APS, and Matter in Extreme Conditions (MEC) endstation at LCLS. In these experiments, postdocs are coupling static compression, mechanical deformation, and shockwave compression (even detonation!) to techniques such as time-resolved x-ray diffraction and scattering, imaging, and x-ray spectroscopies to provide detailed and previously-lacking information about the evolution of materials under the conditions relevant to nuclear weapons. Other postdocs have led research in additive manufacturing and subsequent characterization of the dynamic properties of newly fabricated materials, and novel explosives synthesis and formulation. Postdoctoral research opportunities offer an exciting combination of fundamental science and connection to applied defense missions that are foundational to a research career at the National Laboratories. A high percentage of postdocs within defense programs transition to the technical workforce forming a key pipeline for the future of the Labs.

The **Agnew National Security Postdoctoral Fellow** is one fellowship opportunity at Los Alamos National Laboratory that supports cutting-edge experimental, theoretical, computational science, and engineering research aligned with the Laboratory's national security mission (www.lanl.gov/careers). Thomas Nizolek is a current Agnew Fellow working on in situ temperature and strain mapping during dynamic shear localization within the Materials Science and Technology Division (MST), having joined Los Alamos from an SSAA-funded university research group. Below, Tom describes the drivers for his research and early results from his fellowship appointment.

Dr. Thomas Nizolek is an Agnew National Security Postdoc Fellow in the Materials Science and Technology Division at Los Alamos National Laboratory.

In Situ Temperature and Strain Mapping During Dynamic Shear Localization

T. J. Nizolek, J. A. Valdez, R. M. Martinez, G. T. Gray III

The MST-8 Group at Los Alamos National Laboratory investigates the high strain rate behavior of materials in support of the national security mission. This includes characterizing and predicting the mechanical behavior, equations of state, and failure mechanisms of metals, alloys, actinides, and polymers. While much of this work has historically relied on post-test destructive characterization, new experimental capabilities are enabling in situ measurement of temperature and local strain distributions during

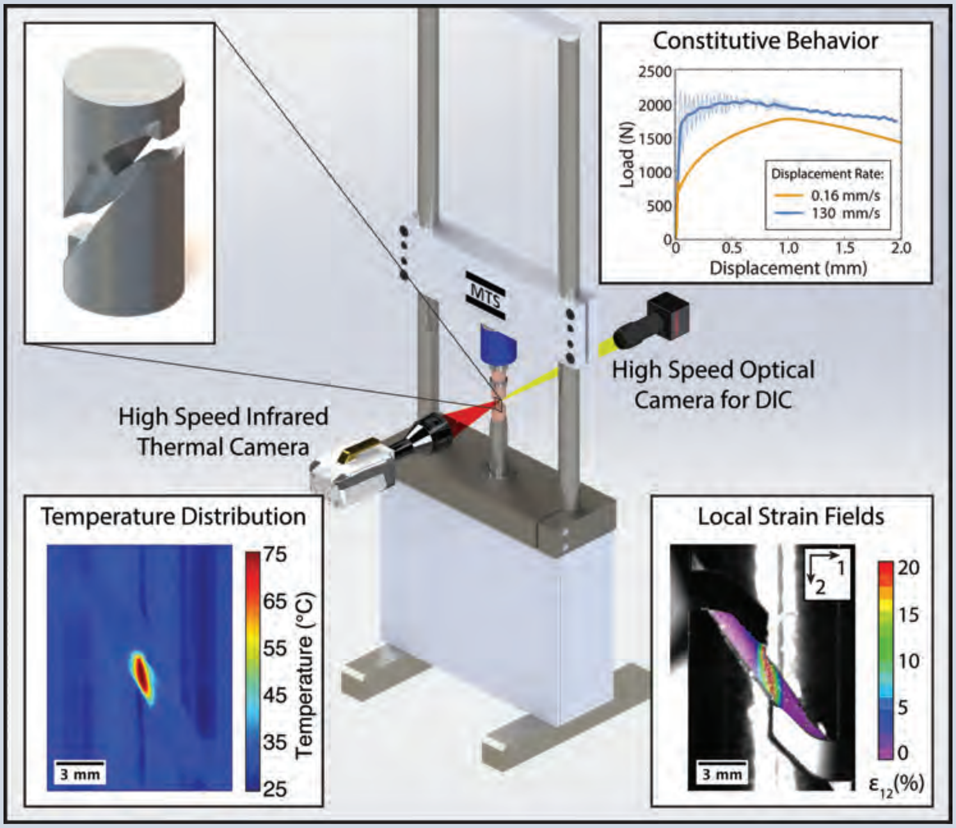


Figure 1. The experimental setup for measuring constitutive behavior, surface temperature distributions, and local strain fields during quasi-static and dynamic shear deformation (heating/cooling chamber omitted for clarity). To generate the highest strain rates, the load frame shown is replaced with a split-Hopkinson pressure bar.

deformation and failure – measurements that will drive the continued development and validation of models for material failure.

Material failure and fragmentation processes are often driven by strain localization, which includes the formation of shear bands.[1] Shear bands result in the breakdown of an initially homogenous deformation field into one containing bands of highly localized shear strain that can serve as sites for damage evolution, crack propagation, and failure. While the basic continuum mechanics framework for shear band formation was developed over 40 years ago,[2,3] numerous materials science questions remain: namely, what is the role of microstructural anisotropy in driving shear localization and to what extent do softening mechanisms such as self-heating and dynamic recrystallization occur and promote localization?

To better understand the effects of microstructure and deformation-induced heating on the propensity for shear localization, we are conducting large-strain shear experiments on high-purity tantalum using a novel shear specimen design. Tantalum is a dense, body centered cubic (BCC) refractory metal of relevance to the defense industry that deforms solely by crystallographic slip (dislocation motion along preferred crystallographic planes) at the strain rates studied in the present experiments.[4] As a single-phase metal with limited and well-characterized deformation modes, tantalum provides an ideal material system in which to study the complex changes in microstructure and constitutive behavior induced by large shear deformation. The shear specimen geometry used in this investigation is based on the compact forced shear specimen design of Gray et al.,[5] but includes several modifications designed to enable in situ observation of the shear region. These specimens possess several advantages[5] compared to conventional shear specimens: 1) they are amenable to a variety of loading platforms, enabling strain rates ranging from 10^{-3} to 10^{4} per second, 2) they provide a simple shear stress state and unique shear plane that can be oriented with respect to an anisotropic microstructure, such as that found in many additively manufactured materials, and 3) they enable in situ observation of the shear zone using a variety of imaging techniques.

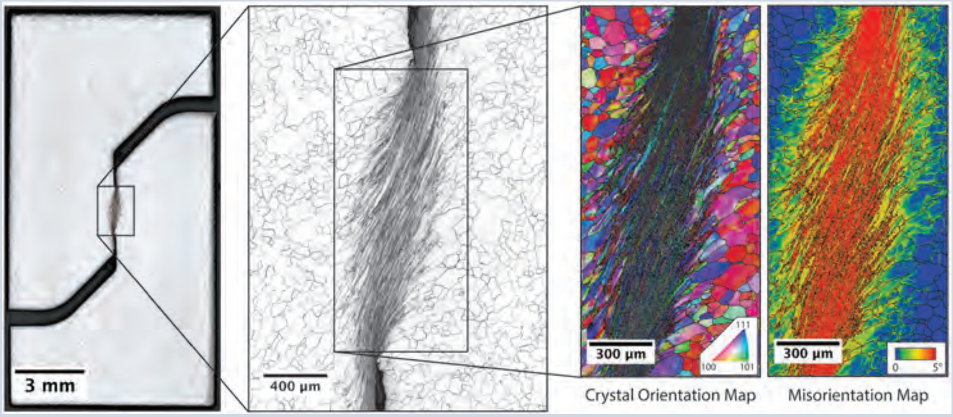


Figure 2: Post-test characterization using optical microcopy and electron backscatter diffraction complements in situ diagnostics by revealing the effects of shear deformation on grain morphology, crystallographic orientations, and the intra-grain misorientation resulting from the accumulation of dislocations.

As shown in Figure 1, the combination of the new specimen geometry, a high-speed infrared camera, and high speed digital image correlation allows for in situ measurement of the surface temperature in the shear zone and the local strain distribution associated with the shear deformation. Further, post-test characterization of the tantalum shear specimens provides insight into the microstructural changes that occur during shear deformation (see Figure 2). These changes include severe elongation of grains in the shear region, crystallographic orientation changes due to slip system activity, and large intra-grain misorientation due to the accumulation of dislocations and damage.

These experimental outputs serve both to test existing models of strain localization[6] and improve future modeling efforts by enhancing our knowledge of the physical processes behind shear localization. The spatially resolved temperature and strain data can be directly compared to results from finite element simulation and, in combination, they ensure that both the kinematics and constitutive behavior of the material in the shear zone is accurately captured. The microstructural changes, including changes in the distribution of crystallographic orientations, provide insight into the physical mechanisms of plastic deformation (dislocation multiplication and slip system activity), thereby improving the physics foundation for crystal plasticity finite element simulations.

By applying new in situ diagnostics and advanced characterization techniques to the complex problem of shear localization, we aim to improve both our fundamental understanding of dynamic shear localization and our capability to predict shear-dominated failure events. It is anticipated that the experimental capabilities developed during the present investigation will enable future studies of materials in which additional deformation mechanisms, such as phase transformation twinning (mechanisms that result in abrupt changes in crystal structure or crystallographic orientation), influence the dynamic shear behavior.

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[2]R. Hill and J.W. Hutchinson, "Bifurcation Phenomena in the Plane Tension Test," J. Mech. Phys. Solids. 23, 239-264 (1975).

[3]J.W. Hutchinson and V. Tvergaard, "Shear Band Formation in Plane Strain. Int. J. Solids Struc. 17, 451-470 (1981).

[4]B.J. Lee et al., "Modeling the Mechanical Behavior of Tantalum," Met. Mater. Trans. A. 28, 113-122 (1997).

[5]G.T. Gray, K.S. Vecchio, and V. Livescu, "Compact Forced Simple-Shear Sample for Studying Shear Localization in Materials," Acta. Mater. 103, 12-22 (2016).

[6]C.A. Bronkhorst et al., "An Experimental and Numerical Study of the Localization Behavior of Tantalum and Stainless Steel," Int. J. Plast. 22, 1304-1335 (2006).

The High Energy Density Physics (HEDP) Summer Student program brings in the most qualified and talented graduate and undergraduate students to work on a diverse collection of research projects. HEDP students are amongst the hundreds that join Lawrence Livermore National Laboratory's ranks each summer to conduct research and take advantage of the rich scientific community it offers.

— Britton Olson, Lawrence Livermore National Laboratory

The Agnew National Security Postdoctoral Fellow is one fellowship opportunity at Los Alamos National Laboratory that supports cutting-edge experimental, theoretical, computational science, and engineering research aligned with the Laboratory's national security mission (www.lanl.gov/careers).

— Dana M. Dattelbaum, Los Alamos National Laboratory

Sandia's research staff works at the forefront of innovation, collaborating in research with universities and companies and pursuing discretionary research projects with significant potential impact. We perform high energy density experiments on the Z facility and other facilities at Sandia and throughout the country, push the forefront of atomistic modeling techniques, and explore material behavior under a wide range of conditions.

— Dawn Flicker, Sandia National Laboratories

Research Opportunities in Support of Stockpile Stewardship in the NNSA Nevada Enterprise

Aaron Luttman, Manager, Diagnostic Research and Material Studies (luttmaab@nv.doe.gov),
Nevada National Security Site

A core mission of the Nevada National Security Site (NNSS), and the NNSA's Nevada Enterprise (NvE) more broadly, is research and development of diagnostic systems to support the National Security Laboratories in Stockpile Stewardship, including subcritical experiments (SCE) in support of certifying the nation's stockpile, fundamental shock physics and dynamic materials research, plasma and nuclear physics, and pulsed-power engineering. Each scientific endeavor requires different measurements and different technical expertise to design the diagnostics. There is a wide range of science and engineering research in the NvE, and here we highlight three exciting opportunities for future graduate student and postdoctoral research in support of national security experiments.

X-ray Detectors at NNSS Livermore Operations

Imaging x-ray emissions is an essential measurement for a wide range of experimental facilities, from inertial confinement fusion laboratories like the Lawrence Livermore National Laboratory's (LLNL) National Ignition Facility (NIF) to linear accelerators like the Stanford Synchrotron Radiation Light Source. Most x-ray photocathodes suffer a sharp reduction in quantum efficiency above 10 keV, limiting our current capabilities and the questions that can be answered. Dr. Kathy Opachich of the NNSS's Livermore Operations is leading a collaboration of researchers from LLNL, Lawrence Berkeley National Laboratory, and industry to design a next-generation photocathode that can provide a 3.5x increase in yield, without compromising

Figure 1. Dr. Kathy Opachich demonstrates her team's novel photocathode design.

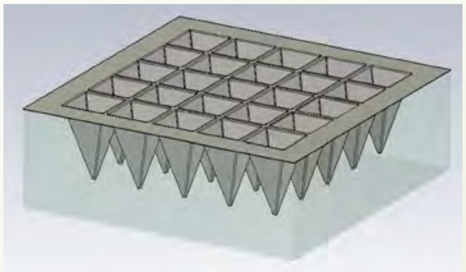

Figure 2. Recessed pyramids photocathode design.

the spatial and temporal performance of the x-ray imagers (see Figure 1). This results in higher-quality imaging up to 10 keV, but also extends our detection capability up to 20 keV, enabling a new class of experiments. The new design exploits the principles that the secondary electron output of an x-ray photocathode is a function of the angle of incidence at which the x-rays hit it and of the material coating the cathode. As the angle of incidence decreases, the electron output increases, so the team moved away from a traditional flat surface to an array of recessed pyramids, where almost all of the x-rays are absorbed at small angles (see Figure 2). While geometrically structured photocathodes had been developed previously, they focused on raised cone or pillar structures, which introduced noise and did not show stable emission properties in high electric fields that are typically present in x-ray detectors. The new approach was so successful that in addition to producing several publications in leading journals, the team was honored with a 2017 R&D 100 Award and received a U.S. government patent on their design. According to Dr. Opachich, "We're really excited about our latest developments, as they are opening up new research directions for the next generation of diagnostic scientists in physics, chemistry, and electrical and nuclear engineering. There are great opportunities for graduate students and postdoctoral researchers to join us in developing measurement systems that will have immediate impact on experiments at NIF, the Stanford synchrotron, and the Advanced Photon Source at Argonne National Laboratory."

Nevada Science Initiative

Understanding the behavior of materials under extreme temperatures and pressures is one of the core scientific thrusts of the NNSA. This research requires laboratories for the experiments, diagnostics to make meaningful measurements, and facilities to develop the diagnostics. The need for facilities whose primary focus is the testing and evaluation of diagnostic systems for dynamic materials research —and the related need to train the next generation of diagnostic scientists and engineers—was the driver for the NNSS to launch the Nevada Science Initiative (NSI), which has established a large-bore propellant launcher (gun) at the NNSS facility in North Las Vegas. High-velocity guns are a common platform for dynamic materials research and for enhancing the diagnostic capabilities that such research requires. The data obtained from gas gun experiments help explain how materials yield in compression and tension, determine shock wave velocities, and clarify dislocation dynamics of materials as they yield, all of which are important to understanding and validating the fundamental physics models used in the large hydrodynamic codes that underwrite our confidence in the nation's nuclear weapons stockpile.

NNSS researchers commissioned the new launcher in North Las Vegas in 2016. The team has begun working with the national laboratories to field fundamental physics experiments, to develop and test new diagnostics for material studies, and to train scientists, engineers, and technicians on how to perform dynamic experiments. Dr. Sarah Thomas joined the NNSS as a postdoctoral researcher, and after 2 years of research, including several experimental campaigns through the NSI, she is now a staff scientist (see Figure 3). As she puts it, "Being a postdoc at the NNSS was great. I got to design my own experiments and serve as a principal investigator at laboratories

Figure 3. Dr. Sarah Thomas demonstrates a mutilated steel alloy target after a spall experiment to help us understand how steel behaves in different solid phases.

Figure 4. Dr. Brady Gall works on the pulsed power driver for the NNSS Area 11 Dense Plasma Focus.

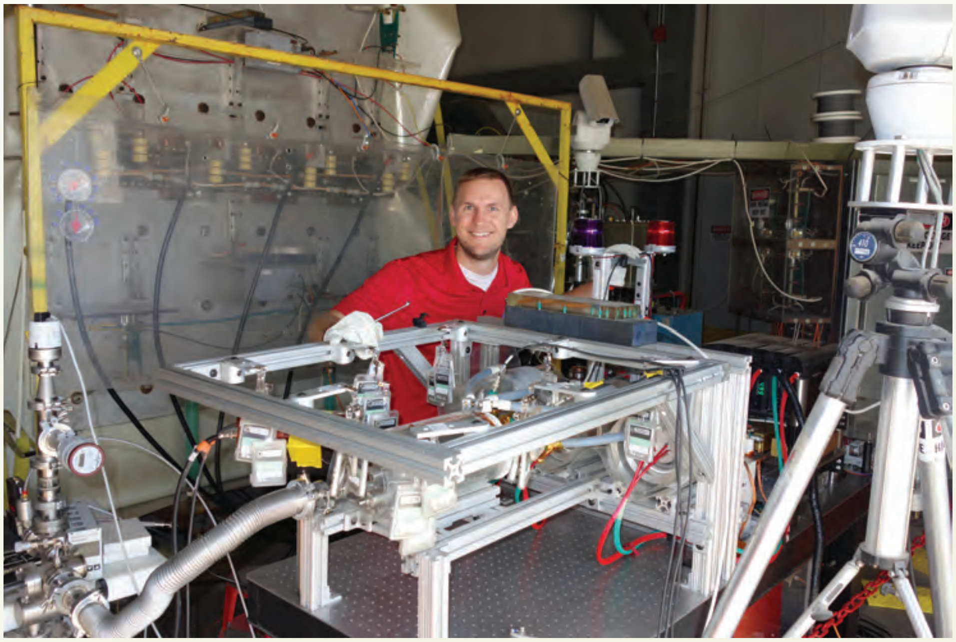

Figure 5. Dr. Gall working on the developmental tabletop DPF, which has applications in both Stockpile Stewardship and Global Security missions.

in Los Alamos, New Mexico, and Santa Barbara, California, as well as at the NSI in North Las Vegas. It was great to see my ideas come to life, leading a great team of experimentalists."

Melissa Matthes came to the NNSS as an intern, which led to her being supported by the NNSS as a graduate student, working in a gas gun laboratory at UNLV. She's now a staff engineer, designing targets and new configurations for the launcher while developing the ability to adjust shot velocity and projectile size. For Melissa, this has been a great experience, "Working on the Nevada Science Initiative has given me the opportunity to understand how to work effectively as a team, to learn from the experts around me, and to contribute my own ideas to stockpile science. Working together, we ensure a successful campaign as a team; even when the experiments have never been done before and we're the ones who have to figure out how to do it."

Pulsed Neutron Source Research

The Nevada National Security Site's U1a Complex is the only facility in the United States where it is possible to carry out high-explosives driven, dynamic plutonium experiments in nuclear weapons relevant geometries, and a research team from the NNSS is supporting Los Alamos National Laboratory (LANL) in the development of a pulsed neutron source for diagnosing the next generation of SCE at U1a. The goal is to measure the nuclear fission decay rate of a subcritical plutonium assembly by pulsing the target with a high flux of neutrons in a short time duration. One of the most direct approaches to generating intense pulses of neutrons is via the fusion of Deuterium (DD) or Deuterium-Tritium gases, and one candidate technology for use on future SCE's is the Dense Plasma Focus (DPF).

> *"There is a wide range of science and engineering research in the Nevada Enterprise, and we're actively seeking enthusiastic graduate students and postdoctoral researchers to play leading roles in solving important problems in national nuclear security."*
>
> *— Dr. Aaron Luttman*
> *Mission Support and Test Services, LLC*

Scientists and engineers at the NNSS and LANL have been collaborating on DPF research for over 15 years, but, in the last 2 years, the pace of DPF development has increased, with a focus on maximizing the neutron yield and controlling the temporal profile of each reaction. This is extremely difficult, since the fusion in a DPF is generally thought to be driven by plasma instabilities, which are, as the name implies, unstable. The team also includes scientists from LLNL and Sandia National Laboratories. DPF offers exciting opportunities for modeling and simulation of pulsed power systems and plasma physics, for the design and development of tritium handling systems, pulsed power drivers, and for developing diagnostics to measure characteristics of the electrical system and the resulting neutron and gamma production.

The lead diagnostics engineer for the multi-mega amp DPF at the NNSS, shown in Figures 4, is Dr. Brady Gall, who is also the principal investigator on a Site-Directed Research and Development project to design and develop a new, modular DPF for portable applications in Global Security. Dr. Gall's team has built a tabletop system, allowing the scientists and engineers working at the NNSS to develop the expertise needed to design and build the next-generation DPF (see Figure 5). According to Dr. Gall, "The Dense Plasma Focus crew is a dynamic mix of recent engineering graduates and experienced plasma source experts, allowing us to incorporate cutting-edge technology into established pulsed power design principles. This unique blend of talent has allowed our team to serve the Stockpile Stewardship and Global Security missions by developing world-class pulsed neutron generators."

The NNSA's Nevada Enterprise is actively working with the National Security Laboratories to develop the advanced diagnostic systems for experiments in support of national nuclear security. There are exciting new opportunities to work with scientists and engineers across the NNSA to design and field cutting edge diagnostic systems used to capture the data needed to ensure the safety, security, and effectiveness of the nation's nuclear weapons stockpile.

Research Opportunities at Sandia National Laboratories

Dawn Flicker (dgflick@sandia.gov) and Mike Cuneo (mecuneo@sandia.gov), Sandia National Laboratories

For more than 60 years, Sandia National Laboratories has delivered essential science and technology to resolve the nation's most challenging security issues. Sandia's research staff works at the forefront of innovation, collaborating in research with universities and companies and pursuing discretionary research projects with significant potential impact. We perform high energy density experiments on the Z facility and other facilities at Sandia and throughout the country, push the forefront of atomistic modeling techniques, and explore material behavior under a wide range of conditions.

Sandia has exciting programs with opportunities in the following areas.

Pulsed-Power Science and Engineering and Accelerator Design

Enabled by the Z Pulsed Power Facility, the world's most powerful pulsed-power accelerator, Sandia's Pulsed Power Sciences Center conducts experiments that achieve unprecedented and extreme states of matter. The Center develops the world's most advanced pulsed-power-accelerator technology and users field experiments in inertial confinement fusion (ICF), materials science, x-ray radiography, weapon effects, radiation physics, laboratory astrophysics, and other areas. There are opportunities to conduct accelerator-physics experiments on Sandia's Z machine, which generates an 85 terawatt 26-megampere 100-nanosecond electrical-power pulse. (The steady-state electrical-power-generating capacity installed worldwide is 5 terawatts.) Z is - by far - the world's largest and most powerful pulsed-power accelerator. Sandia also has several smaller, and more accessible research accelerators. In addition to conducting accelerator-physics experiments, Sandia's Pulsed Power Sciences Center develops mathematical models of pulsed-power components, systems, and accelerators, and perform analytic calculations and numerical simulations.

Radiation Magneto-Hydrodynamics/ Nuclear Astrophysics

Sandia's radiation magneto-hydrodynamics and nuclear physics research contributes to the lab's ICF program and to models that test and predict how materials and systems respond to extreme radiation. The program researches radiation and diffusive transport, magnetically-driven plasma instability growth, and the effects of magnetic fields on fundamental transport properties. Fusion research focuses on Magnetized Liner Inertial Fusion (MagLIF), which combines powerful magnetic fields with laser preheating to generate significant fusion yields on the Z machine. Fundamental research is also being performed in radiation and diffusive transport, magnetically driven plasma instability growth, and the effects of magnetic fields on fundamental transport properties including charged particles in fusing plasmas.

Atomic Physics and Spectroscopy

Atomic physics and applied spectroscopy contribute to Sandia's High Energy Density (HED) Science and ICF programs and include theoretical, computational, and experimental activities. Spectroscopy is among the most powerful diagnostics available to probe HED plasma conditions at the smallest spatial and temporal scales and under the hottest and densest conditions. It also has directly measured plasma electric and magnetic fields, plasma spatial structure, and plasma fusion conditions such as densities, temperatures, impurity mix, and other properties. There is a strong theme of atomic physics and spectroscopy in the Z fundamental science program, which permits university research on the Z facility.

Atomic physics research focuses on atomic processes in dense plasmas, including effects on ionization, energy level structure, and spectral line shapes. Researchers test predictions against data from HED facilities. Z machine experiments study plasma opacity at stellar interior conditions, photoionized plasmas like those found around black holes, and plasma density's effects on spectral line shapes observed from white dwarf stars.

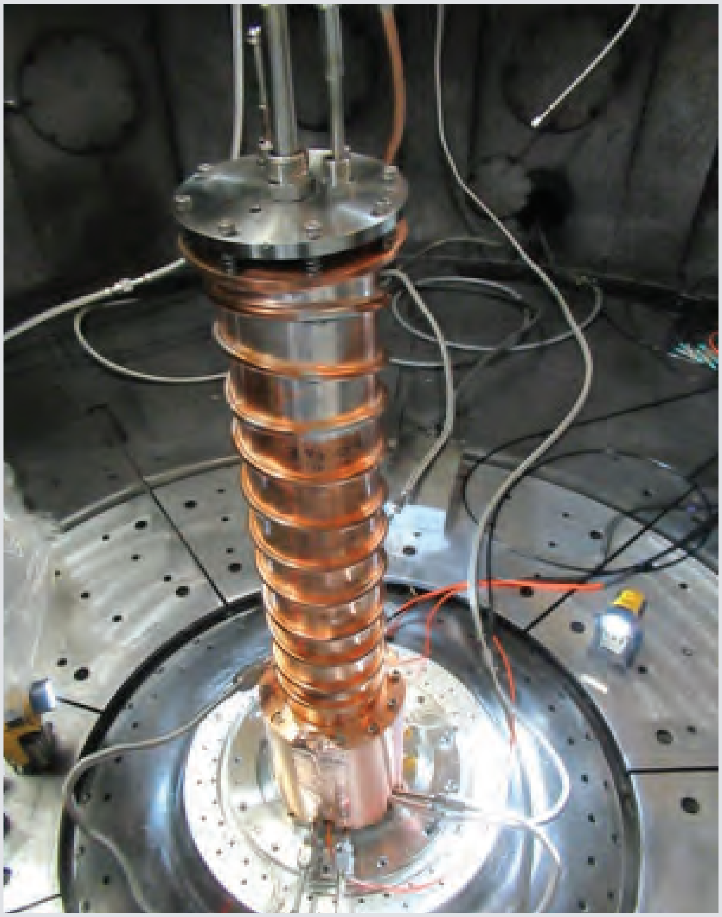

Figure 1. A cryostat used to cool liquid helium to 3.8 K, installed in Z center section.

Visible and x-ray spectroscopy is a key diagnostic for determining plasma characteristics. The Pulsed Power Sciences Center has a world-leading capability to measure and interpret spectra from ICF and HED plasmas. Researchers also work with the international spectroscopy community to advance instrumentation.

Dynamic Materials/Shock Physics

HED material physics researchers employ and develop experiments and theoretical methods to study matter under extreme conditions. The resulting data help understand the structure of Earth and giant planets, planetary impacts, and HED and ICF experiments. Researchers develop temperature and x-ray diffraction diagnostics and a pre-compression cell capability for Z; phase-transition kinetics experiments on the new intermediate scale THOR facility; and time-resolved x-ray diffraction of dynamic compression at Argonne National Laboratory's Advanced Photon Source. Theoretical research centers on advanced methods for calculating phase transitions in solids, transport properties of matter under extreme conditions, and equation of state tables. There is a strong theme of dynamic materials and shock physics in the Z fundamental science program, which permits university research on the Z facility.

In addition to the experimental capabilities, our dynamic material properties program has a distinguished record of collaborative efforts between experiments and corresponding ab initio calculations, principally those with density functional theory (DFT). Theory is used in direct simulation of experimental conditions achieved on Z and other platforms and these calculations have been critical to developing high-fidelity physics models for the design and simulation of Z experiments. Parallel to applying DFT, we also rely on Quantum Monte Carlo (QMC), an advanced method for calculating properties of materials based on the electronic structure of the material. The dramatic increase in computational capabilities available at Sandia has made QMC a viable method for calculating properties of real materials.

Material Science

Foundational materials work at Sandia involves research ranging from the design and synthesis of new materials for specific functionality, developing and prototyping manufacturing processes, applying deep understanding of materials' reliability and failure mechanisms, resolving resolve issues that arise in materials applications, to developing the theoretical and computational insights that enable better life cycle predictivity of materials' performance. Materials of interest include organic materials and composites, glasses and structural and electronic ceramics, and structural metals and metallurgical joining processes such as welding, brazing, and soldering.

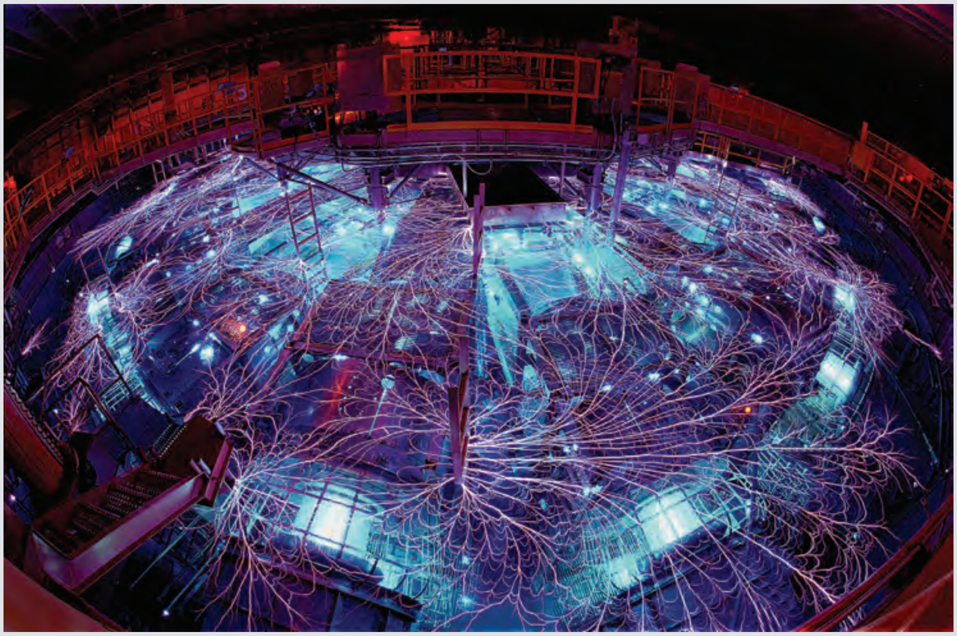

Figure 2. Z machine firing.

Comments from Sandians Who Came from the SSAA Community

"The unique educational opportunities of NNSA's HPCAT and HiPSEC gave me a solid foundation in my training as a materials' and high-pressure physicist. Now, the nurturing environment of Sandia, together with the outstanding expertise of my Sandia colleagues and mentors and access to unparalleled scientific capabilities, are allowing me to embrace confidently a new research field—shock physics—and work towards making my own mark in it."

– Patricia Kalita

"My experience as a staff member at Sandia has been incredibly rewarding due to the combination of outstanding colleagues and superlative resources. However, prior to my interactions with SSAA, I was completely unaware of the opportunities at the labs. Learning about the national laboratories was perhaps one of the most valuable experiences from my postdoctoral career."

– Luke Shulenburger

"While in graduate school I completed an SSGF practicum at Sandia National Laboratories working on power flow in the Z machine. The work was so interesting that I ended up shifting the focus of my graduate research to continue studying the problem. A combination of the connections that I made during the practicum and the general interest in the power flow problem at Sandia ultimately lead me to my current position at the lab."

– Matthew Gomez (see article on p. 48)

"The SSAP program was a great way to introduce myself to lab staff, and directly led to my postdoctoral position at Sandia. My postdoctoral career at Sandia has been an incredible experience thus far. I've been introduced to a wide array of interesting problems, and have enjoyed the opportunity to learn new techniques and collaborate with staff. In particular, I have greatly enjoyed the interactions between theory and experiment, which has certainly amplified the scientific impact of my work."

– Joshua Townsend

List of Grants and Cooperative Agreements

Stewardship Science Academic Alliances

High Energy Density Physics

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

Ohio State University
Douglass Schumacher / Richard Freeman
High Energy Density Physics Program at the Scarlet Laser Facility

University of Nevada, Reno
Alla Safronova
Radiation from High Energy Density Pulsed Power Plasmas and Applications

University of Rochester
Mitchell Anthamatten
Development of Thiol-Ene Networks for Low Density Foams at Cryogenic Conditions

University of Texas at Austin
Todd Ditmire
University of Texas Center for High Energy Density Science

Low Energy Nuclear Science

Colorado School of Mines
Uwe Greife
High Precision Fission Studies with the NIFFTE Fission Time Projection Chamber

Duke University
Calvin Howell
Photo-Fission Product Yields of Special Nuclear Materials

Duke University
Werner Tornow
Neutron-Induced Fission Studies and Reactions on Special Nuclear Materials

Indiana University
Romualdo deSouza
Development of a High-Resolution Position Sensitive MCP-PMT Detector

Michigan State University
Paul Mantica
Pulsed Laser Techniques Applied to Rare Isotopes

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

Michigan State University
William Lynch
Asymmetric Nuclear Matter Under Extreme Conditions

Michigan State University
Witold Nazarewicz
Microscopic Description of the Fission Process

Mississippi State University
Anatoli Afanasjev
Microscopic Description of Fission in a Relativistic Framework

Ohio University
Carl Brune
Studies in Low Energy Nuclear Science

Oregon State University
Walter Loveland
The Energy Release in the Neutron Induced Fission of ^{233}U, ^{235}U, and ^{239}Pu

Rensselaer Polytechnic Institute
Yaron Danon
Experiments with Neutron Induced Reactions

Rutgers University
Jolie Cizewski
Center of Excellence for Radioactive Ion Beam Studies for Stewardship Science

San Diego State University
Calvin Johnson
Ab Initio Calculations of Neutron-Capture Reactions on Light Nuclei

University of Kentucky
Michael Kovash
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Carnegie/DOE Alliance Center: A Center of Excellence for High Pressure Science and Technology

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Massachusetts Institute of Technology
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Warren Mori
Continuation of the Application of Parallel Kinetic Simulations to Laser and Electron Transport Through High Energy Density Laboratory Plasmas

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Chand Joshi
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Alla Safronova
Line Emission from High-Z Multiple Ionized Ions Influenced by Dielectronic Recombination and Polarization

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General Atomics
Mingsheng Wei
Hot Electrons from Nonlinear Plasma Interaction in Shock Ignition Regime

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

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HEDP Explorations of Kinetic Physics, Plasma Stopping Power, Hohlraum Fields and Nuclear Astrophysics

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Laser-Based Dynamic Compression of High-Pressure and Planetary Materials

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Dynamics of Magnetic Reconnection in High-Energy-Density Plasmas

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Study of Magnetized Collisionless Shocks in Laser-Produced Plasmas

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High Energy Density Chemical Physics and Planetary Evolution

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Transport of Reativistic Electrons in Cylindrically Imploded Magnetized Plasmas

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Properties of Magnetohydrodynamic Turbulance in Laser-Produced Plasmas

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Experimental Astrophysics on the OMEGA Laser

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Investigations of Relativistic Reconnection Using OMEGA EP

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Development of a Photoionized Plasma Experiment at OMEGA EP

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Gianluca Iaccarino
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Center for Exascale Radiation Transport

The University of Utah
Philip J. Smith
Carbon Capture Multidisciplinary Simulation Center

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LABORATORY RESIDENCY GRADUATE FELLOWSHIP

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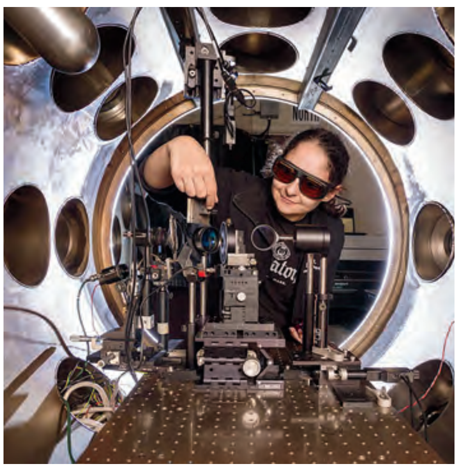
LABORATORY RESIDENCY GRADUATE FELLOWSHIP



Top: The rendering of the inside of NIF's target chamber shows the target positioner moving into place. Pulses from NIF's high-powered lasers race through the facility at the speed of light and arrive at the center of the target chamber within a few trillionths of a second of each other, aligned to the accuracy of the diameter of a human hair. Courtesy of Lawrence Livermore National Laboratory.

Bottom: Postdoc S. Ali adjusts a target in the Janus laser at Livermore's Jupiter Laser Facility.

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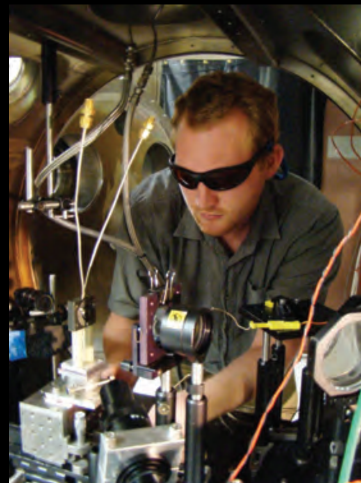
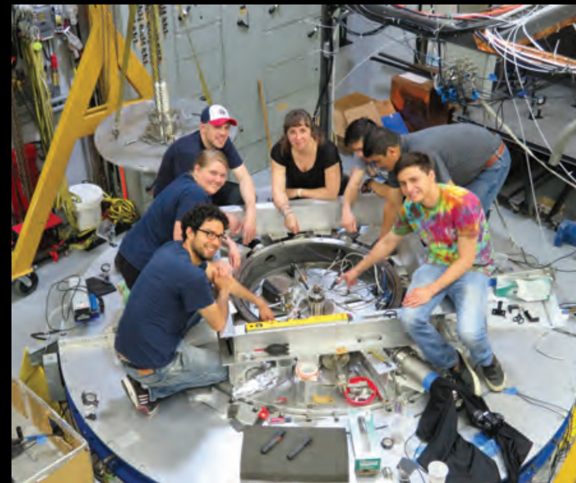

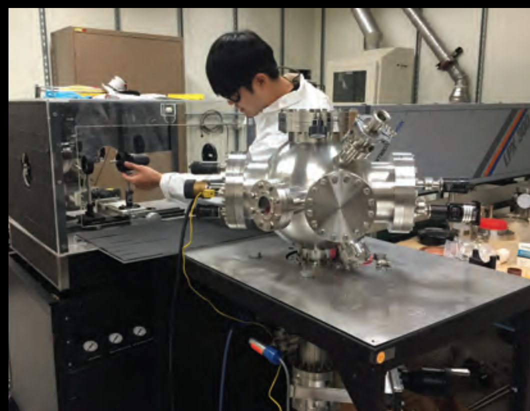


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