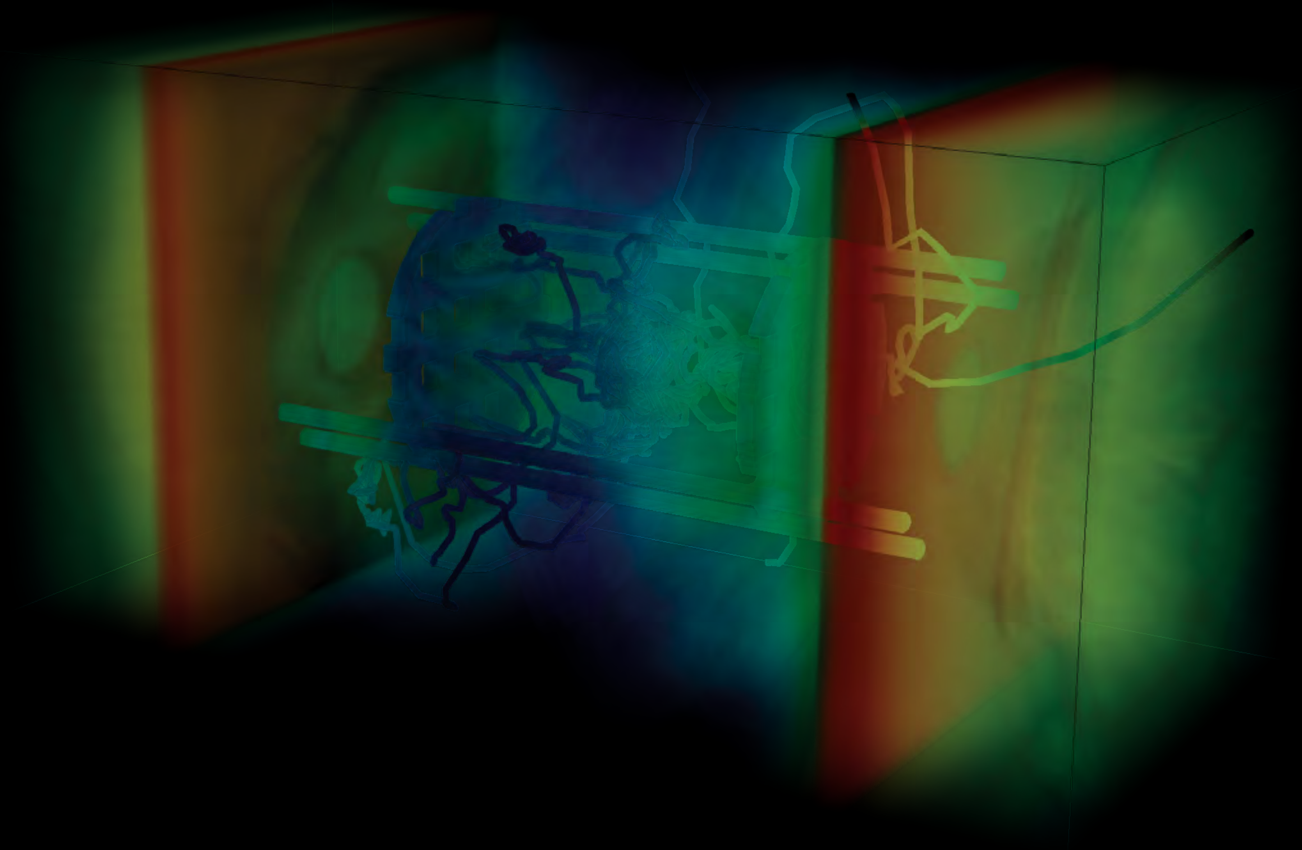
DOE/NA-0056

2017
Stewardship Science Academic Programs Annual

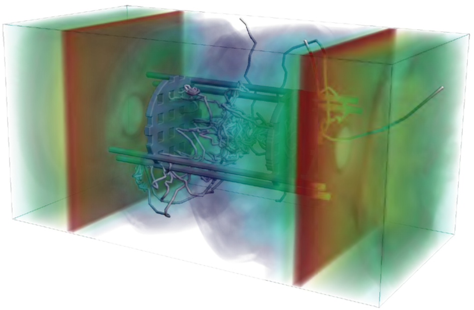
- Stewardship Science Academic Alliances
- High Energy Density Laboratory Plasmas
- National Laser Users' Facility
- Predictive Science Academic Alliance Program II



National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY

On the Cover



The Turbulent Dynamo (TDyno) National Laser Users' Facility (NLUF) campaign utilizes the Omega-60 laser at the University of Rochester Laboratory for Laser Energetics to demonstrate and study one of the greatest puzzles of modern astrophysics: the amplification of magnetic fields by the turbulent dynamo mechanism, a ubiquitous process in the universe that can explain the observed values of cosmic magnetic fields. The cover image shows a three-dimensional (3D) radiation magneto-hydrodynamic simulation of the experimental platform, performed with the multi-physics code FLASH on the Mira BG/Q supercomputer at Argonne National Laboratory. Shown is a 3D rendering of the plasma density: the Omega driver beams illuminate two foil targets (in red) to create counter-propagating flows that traverse a pair of grids (gray contours) and collide to form a hot, turbulent plasma at the center. The seed magnetic fields generated by the laser-target interaction are amplified by the turbulent dynamo mechanism to reach values close to equipartition with the kinetic energy of the turbulence. The white, tangled lines are sample magnetic field lines in the turbulent region.

Image courtesy of Dr. D. Lamb, University of Chicago

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2017 Stewardship Science Academic Programs Annual

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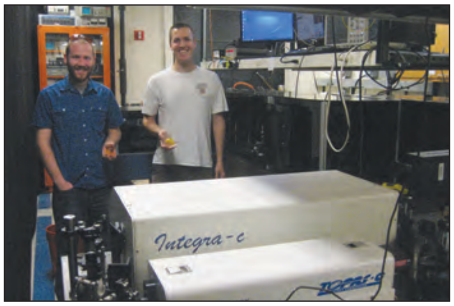

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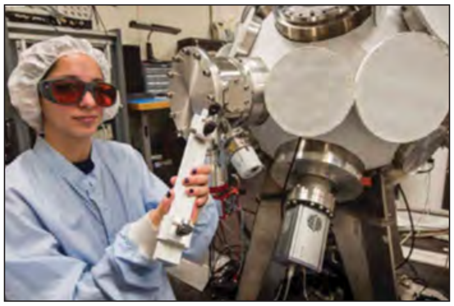

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Welcome from the Assistant Deputy Administrator for Research, Development, Test, and Evaluation

One of the primary missions of NNSA is to ensure a safe, secure, and effective nuclear deterrent without nuclear explosive testing. NNSA and its national laboratories have developed a science-based Stockpile Stewardship Program (SSP) to maintain and enhance its scientific, engineering, and computational capabilities to sustain the ability to assess and certify the stockpile in the absence of nuclear testing.

Training people to maintain and refresh specialized scientific and engineering expertise and skills in essential areas are critical to ensuring the integrity of the nuclear deterrent. NNSA developed the Stewardship Science Academic Programs (SSAP) more than a decade ago to provide the future capability for stockpile stewardship by supporting students and their professors to develop the technical skills required of future stewards of the stockpile. The SSAP are essential to maintaining a pipeline of professionals to support the technical capabilities that reside at the NNSA national laboratories, sites, and plants. We are pleased that many past participants from the SSAP have chosen a career with the NNSA national laboratories. These talented scientists and engineers are an important part of our current and projected future success.

The high quality of the work performed under the SSAP is clearly reflected in this 2017 Stewardship Science Academic Programs Annual. The work presented herein, however, represents only a fraction of the outstanding work done in the SSAP to provide an excellent pipeline of talent and new ideas relevant to stockpile stewardship.

As we look to the future, science-based SSP will continue to be core to NNSA's nuclear mission with SSAP playing a pivotal role in ensuring that future. To all of you participating in the SSAP, I extend my best wishes for your continued success and congratulations on your successes to date.

Dr. Kathleen B. Alexander

Assistant Deputy Administrator
for Research, Development, Test,
and Evaluation

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The Nation's nuclear weapons stockpile is a vital part of our national security infrastructure. Ensuring that this deterrent is unequaled 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).

The 2016-2017 SSGF fellows took time during the SSGF Annual Meeting to pose for a class photograph. Left to right: Viktor Rozsa, Benjamin Musci, Heather Sandefur, Miguel Holgado, Daniel Woodbury, and Cody Dennett. Not pictured: Erin Good.

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.

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 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.

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.

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.

Dr. Sarah Wilk, Program Director for the NNSA Stewardship Science Academic Alliances addresses attendees of the Poster Session of the Stewardship Science Graduate Fellowship Annual Program Review in Las Vegas on June 27, 2016.

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.

DOE/NNSA Graduate Fellowship Programs

Also a part of the SSAP are 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. These 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.

The NNSA Office of Research, Development, Test, and Evaluation manages the SSAP. To learn more about this office, visit www.nnsa.energy.gov/stockpilestewardship.

Stewardship Science Academic Alliances (SSAA): Supporting National Security

Interview with Dr. Sarah Wilk, SSAA Program Director

What is the purpose of NNSA's SSAA Program?


Sarah Wilk

The Stewardship Science Academic Alliances (SSAA) Program was established in 2002 to support state-of-the-art research at U.S. academic institutions in areas of fundamental physical science and technology of relevance to the Stockpile Stewardship Program (SSP) mission, such as: materials science, high energy density physics, radiochemistry, and low energy nuclear science.

How is the SSAA Program vital to stockpile stewardship?

The SSAA Program provides the research experience necessary to maintain a cadre of trained scientists at U.S. universities to meet the Nation's current and future SSP needs, with a focus on those areas not supported by other federal agencies. It supports the DOE/NNSA's priorities both to address the workforce-specific needs in science, technology, engineering, and mathematics and to support the next generation of professionals who will meet those needs.

How do the disciplines supported by the SSAA Program serve national security?

Since 1992, the United States has observed the moratorium on underground nuclear testing. Therefore, research and development activities are essential to maintain the safety, security, and effectiveness of the Nation's nuclear weapons stockpile. This nuclear deterrent remains a vital part of our national security infrastructure. The four technical areas mentioned above are critical to the SSP, and maintaining a well-trained pipeline of new scientists conducting world-class research in these areas supports our national security. Additionally, many of these skills benefit other DOE/NNSA national security missions such as nuclear nonproliferation and counterterrorism.

What unique academic experiences, insights, and skillsets do you bring to managing the SSAA Program?

As a nuclear chemist, much of the training you receive and research you do is relevant to matters of national defense and security, whether directly or indirectly. My late adviser Heino Nitsche was an SSAA recipient, and though my doctoral research was not funded through his SSAA award, I was able to witness the research being done by those on the project. In addition to nuclear chemistry, I have conducted research in other fields such as materials science and neutron physics.

Away from the bench, I worked for three and a half years on assignment at the Defense Threat Reduction Agency with their Basic and Applied Research Department, which funds academic research in very similar technical disciplines to SSAA. There I worked in the areas of nuclear forensics and nuclear nonproliferation, putting out numerous calls for proposals, reviewing applications, and making funding recommendations. This experience was excellent preparation for working with the SSAA Program, and I will combine that experience with my broad technical background in the role of Program Director.

As the Program Director, what are your immediate goals for the SSAA Program?

My first goal has been realized – the release of our Funding Opportunity Announcement for SSAA Centers of Excellence, mentioned below. My further goals include a call for SSAA academic grants late in the year, and examining the history and successes of the Program to ensure it is working well for all parties.

Has the SSAA Program been successful? How is that success measured?

The SSAA program has indeed been successful, with more than 250 students hired by the NNSA national laboratories or other U.S. Government agencies. In addition, more than 4,500 publications have resulted from SSAA-funded research, representing a substantial contribution to our scientific body of knowledge. (All numbers current as of the time this article went to press.)

When is the next call for proposals for the SSAA Program?

The Program has an open call for our next cohort of SSAA Centers of Excellence which closes April 30, 2017. A Center is made up of a team of academic partners that performs exciting, creative, and challenging research in a topical research area in a collaborative manner. For more detailed information please refer to grants.gov, Funding Opportunity Announcement: DE-FOA-0001634.

How can someone submit ideas to help improve the SSAA Program?

I am always interested in hearing ways to improve our Program. Please feel free to contact me with any suggestions you may have at sarah.wilk@nnsa.doe.gov.

> *“The SSAA program has indeed been successful, with more than 250 students hired by the NNSA national laboratories or other U.S. Government agencies. In addition, more than 4,500 publications have resulted from SSAA-funded research, representing a substantial contribution to our scientific body of knowledge.”*
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> *— Dr. Sarah Wilk, Program Director, SSAA*

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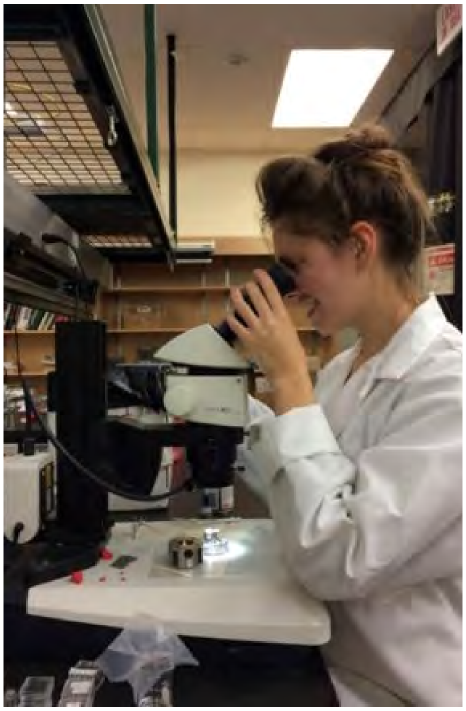

Stewardship Science Academic Alliances

New Developments at Carnegie-DOE Alliance Center

Carnegie Institution of Washington ❖ Director: Russell J. Hemley (rhemley@email.gwu.edu); Coordinator: Stephen A. Gramsch (sgramsch@carnegiescience.edu)

Now in its fourteenth year as a Center of Excellence for High Pressure Science and Technology within the NNSA Stewardship Science Academic Programs, the Carnegie-DOE Alliance Center (CDAC) has as its mission to expand the understanding of materials behavior at extreme pressure-temperature (*P-T*) conditions, develop new facilities and methods to advance high *P-T* materials research, and support the education and training of graduate students for work in areas of importance to Stockpile Stewardship.

Scientific Program and Structure

Since its founding in 2003, the CDAC scientific program has been divided broadly into six primary areas of research:

1. High *P-T* Phase Relations and Structures,
2. *P-V* (volume)-*T* Equations of State,
3. Phonons, Vibrational Thermodynamics and Elasticity,
4. Plasticity, Yield Strength and Deformation,
5. Electronic and Magnetic Structures and Dynamics, and
6. High *P-T* Chemistry.

CDAC consists of a core group of scientific and technical personnel at the Carnegie Institution in Washington, DC along with 14 academic partners and the students they support through CDAC (19 during the current year), and a group of NNSA Laboratory Partners, consisting of individuals representing the extreme conditions research groups at the NNSA national laboratories.

Recent Highlights

Theory

Founded mainly as an experimental program, theoretical work now plays an increasingly important role in many CDAC groups. From the prediction of crystal structures of high pressure phases using first-principles electronic structure methods to the development of special techniques for modeling texture development in two-component samples at pressure, the variety of computational tools employed by CDAC researchers continues to grow.

In its third phase, starting in 2013, CDAC added as an Academic Partner Professor Eva Zurek, from the Chemistry Department, University at Buffalo. Her research focuses on the prediction of novel structures at extreme conditions and studies of structure-property relationships in molecules and solids. Through her collaborations with the Quantum Simulations group at Lawrence Livermore National Laboratory (LLNL), Professor Zurek's wide range of scientific interests helps strengthen the ties between CDAC and the NNSA laboratories.

At Carnegie, the computational aspect has also been strengthened by the participation of Research Scientist Ivan Naumov, who focuses on the fundamental physics of elemental systems at extreme conditions. Most recently, Naumov and his team have discovered remarkable similarities in the electronic structures of molecular hydrogen and lithium at very high pressures, and predicted the existence of surface superconductivity in dense hydrogen. These results are contributing to related studies currently ongoing at the NNSA Laboratories.

Shock Compression in CDAC

One of the continuing goals of CDAC has been bridging the gap between static and dynamic compression. Previously, CDAC allocated beam time at the CDAC-supported synchrotron beamline U2A at the National Synchrotron Light Source (NSLS), to a group from Sandia National Laboratories to carry out the first shock compression studies at a synchrotron facility. Subsequently, CDAC beam time was made available at the HPCAT facility at the Advanced Photon Source (APS), for the first x-ray diffraction measurements of shock-compressed materials. The latter experiments set the stage for the Dynamic Compression Sector (DCS) at the APS, now in its commissioning phase. Current and former CDAC Academic Partners are now active users of DCS. In addition, CDAC is leading two discovery science campaigns at the National Ignition Facility (NIF).

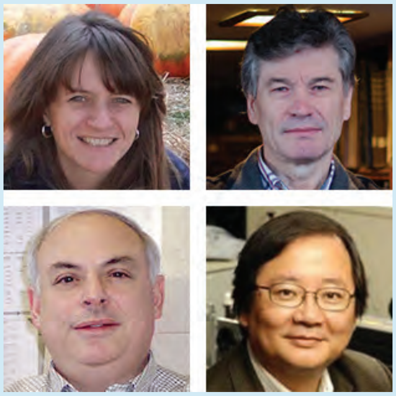

Figure 1. CDAC Scientists. Clockwise from upper left: CDAC Academic Partner Eva Zurek (Buffalo), CDAC Research Scientist Ivan Naumov (Carnegie), CDAC Academic Partner Dana Dlott (Illinois), and CDAC Academic Partner Choong-shik Yoo (Washington State).

With CDAC support, the research group of Academic Partner Dana Dlott of the University of Illinois (see Figure 1) has developed a shock wave spectroscopy apparatus that uses Doppler velocimetry to monitor the launch, flight and impact of flyer plates with selected sample materials. The apparatus has been interfaced with spectroscopic tools and can now launch 100 flyer plates per day, with excellent reproducibility. Using the flyer plate apparatus, graduate students Will Shaw and Will Bassett (see Figure 2) have investigated the shock initiation of energetic materials. Thus far, the emission data obtained agree well with optical measurements, but the flyer plate apparatus offers superior dynamic range and nanosecond time resolution. Will Shaw is the latest addition from CDAC to the NNSA Laboratories, having joined LLNL in September 2016.

Using CDAC beam time at HPCAT, CDAC Academic Partner Choong-shik Yoo of Washington State University (see Figure 1) explores the kinetics of solid-solid transitions using the dynamic diamond anvil cell (d-DAC). The d-DAC allows precise control of pressure and compression rates, and when coupled with time-resolved synchrotron x-rays, Raman spectroscopy, and microphotography, offers a unique method for studying transformations that would not be accessible using static methods alone. Initial experiments by CDAC graduate student Dane Tomasino

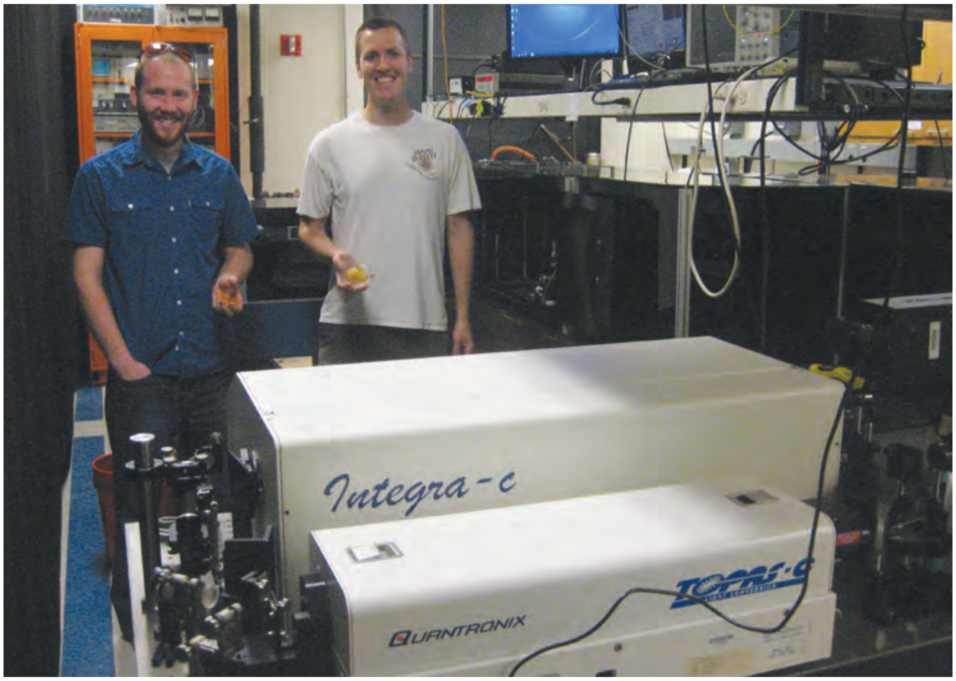

Figure 2. CDAC graduate students Will Shaw (left) and Will Bassett with the flyer plate apparatus in their laboratory at Illinois.

> *"... CDAC has as its mission to expand the understanding of materials behavior at extreme pressure-temperature (P-T) conditions, develop new facilities and methods to advance high P-T materials research, and support the education and training of graduate students for work in areas of importance to Stockpile Stewardship."*

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using the d-DAC include time-resolved synchrotron x-ray diffraction studies of the structural evolution of H_2O across a series of phase boundaries over a broad range of compression rates. Equations of state determined using the d-DAC agree well with static measurements carried out with standard DAC methods.

CDAC Student Enrichment at NNSA Laboratories

Over the past three years, CDAC has supported the attendance of graduate students at the NNSA national laboratories for summer internships that have significantly enriched their dissertation research (see Figure 3). Eloisa Zepeda Alarcón (UC-Berkeley/Hans-Rudolf Wenk) and Andrew Shamp (Buffalo/Eva Zurek) visited Los Alamos National Laboratory (LANL) and LLNL, respectively in the summer of 2014. Eloisa worked in the Materials Science in Radiation and Dynamics Extremes Group with R. Lebensohn and C. Tome on viscoplastic modeling of two-phase aggregates of minerals. This has provided a valuable supplement to her experimental work at Berkeley on plastic deformation and texture development in minerals at pressures relevant to Earth's deep mantle. In the Quantum Simulations Group at LLNL, Andrew collaborated with E. Schwegler, S. Hamel, and T. Ogitsu on the development of *ab initio* molecular dynamics methods for the study of materials at pressures relevant to those achieved during laser shock compression at the NIF. As a result, Andrew's previous work on boron carbide at extreme conditions, carried out mainly with density-functional methods, can be extended into much higher *P-T* regimes.

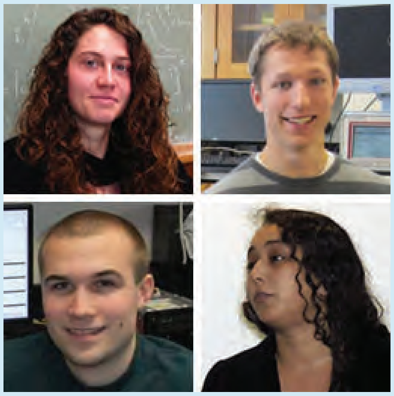

Figure 3. CDAC graduate students participating in NNSA laboratory internships. Clockwise from upper left: Jane Herriman (Caltech), John Lazarz (Northwestern), Eloisa Zepeda-Alarcón (UC-Berkeley), and Andrew Shamp (Buffalo).

During the summer of 2015 and for several months following, John Lazarz (Northwestern/Steven Jacobsen) visited LANL to work in the Shock and Detonation Physics Group with K. Ramos, C. Bolme, and D. Hooks. John upgraded the group's Brillouin spectrometer to be compatible with high-pressure diamond anvil cell measurements and rebuilt a petrographic microscope/spindle stage assembly. He then used the apparatus to measure the complete optical indicatrix of acetaminophen (a proxy for explosives) in order to be able to interpret Brillouin scattering data on sound velocities. Finally, Lazarz was able to measure for the first time the complete elastic tensor for this important material.

Jane Herriman (California Institute of Technology/Brent Fultz) participated in the Computational Chemistry and Materials Science Summer Institute at LLNL in the summer of 2016, and with CDAC support, will be extending her stay through the completion of her dissertation work. Herriman's work in the Quantum Simulations Group on high performance computing and molecular dynamics has been carried out in collaboration with E. Schwegler, X. Andrade, and E. Draeger.

The Effects of Material Strength on Rayleigh Taylor Turbulence

Lehigh University ❖ PI: Arindam Banerjee (arb612@lehigh.edu)

The Turbulent Flow Design Laboratory at Lehigh University has been performing novel experimental research on Rayleigh Taylor instability (RTI). For the past four years, support from the Stewardship Science Academic Alliances (SSAA) program has allowed the principal investigator (PI) to conduct two extensive RT experimental studies in elastic plastic materials, and under variable acceleration histories. The data sets from these experiments are being used by SSAA members for code validation and model development. Currently, SSAA supports two doctoral students who are working on experiments at Lehigh University. A third doctoral student is currently working with Daniel Livescu at Los Alamos National Laboratory (LANL) performing direct numerical simulations of the RT variable acceleration problem.[1] According to PI Arindam Banerjee, “Support from the NNSA has allowed me to provide students with the necessary laboratory experience and the opportunity to learn about computations at DOE national laboratories. Being a SSAA alum myself, I believe that the program is providing students opportunities for high quality and well-rounded research and educational experience in areas of national need.”

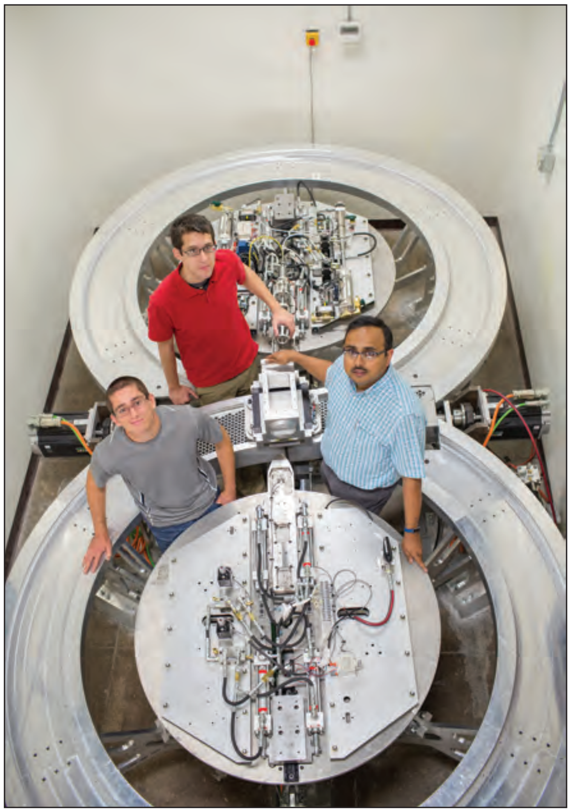

Figure 1.The rotating Wheel RT Experimental Facility at Lehigh.

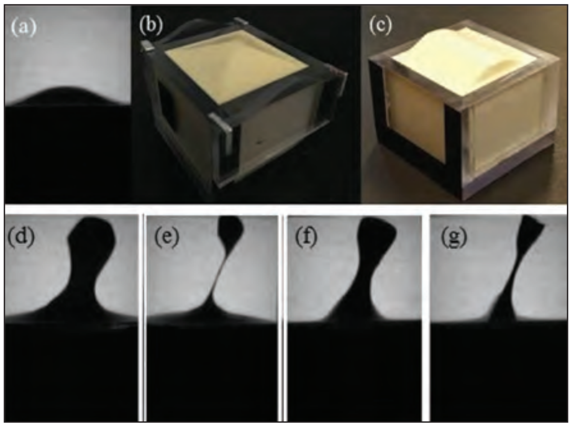

Figure 2. (a) Backlit image of test section at the start of the experiment; (b) initial perturbation 3D interface. (c) Initial perturbation 2D interface (both with wavelength = L, amplitude = L/15); (d)-(e) instability evolution for 3D interface with wavelengths L/2 and L/4; (f)-(g) instability evolution for 2D interface with wavelengths L/2 and L/4 (L = test section width = 60 mm).

RTI occurs between materials of dissimilar densities when the density and pressure gradients are in opposite directions, creating an unstable stratification. In situations (e.g., high-energy applications) where one or both of the materials involved is a solid rather than a liquid, material strength has a significant effect in suppressing mixing. The understanding of RT in accelerated solids has been limited because instability evolution is governed by the nonlinear constitutive equations that describe the elastic-plastic (EP) properties for solid materials that exhibit both viscous and elastic characteristics under deformation. Experimental investigation of the phenomena is challenging due to the exceedingly small time scales and large measurement uncertainties of material properties. Scaled experiments of RTI in elastic-plastic materials using emulsion (mayonnaise) are being conducted to complement laboratory experiments at high pressure because a higher precision is possible as constitutive properties are better known and parameters can be easily varied.

For this purpose, a rotating wheel RT experiment has been developed at Lehigh (see Figure 1) which allows for large/variable accelerations to study RTI in both liquids and EP solids. In the last calendar year, our research has focused on RT experiments in solids, more notably investigating the instability threshold. Various interfacial perturbations, two- and three-dimensional (2D and 3D) with varying amplitude/wavelength, were compared to study the acceleration required for instability and the exponential growth after the interface yielded; the 3D interfaces were found to be more stable than the 2D counterparts (see Figure 2). A decrease in initial amplitude produced a more stable interface that increased the threshold acceleration required for the instability. Exponential growth rates were observed after instability was reached with trends of increasing growth rates for lower initial amplitudes. Critical amplitude conditions for instability were calculated and compared with experimental results and various analytical models to evaluate viscosity at these high strain-rates.[2]

References

[1] Non-Boussinesq Effects on Buoyancy Driven Variable Density Turbulence, Denis Aslangil, Daniel Livescu, and Arindam Banerjee, 69th American Physical Society, DFD Abstract # M34.00006, Portland, Oregon, 2016.

[2] Arindam Banerjee, Rinosh Polavarapu, and Pamela Roach, “Rayleigh-Taylor Instability Experiments with Elastic Plastic Materials,” submitted to Physical Review E, 2017.

New Multimodal Characterization of Additive Structures for Extreme Environments

University of California, Santa Barbara ❖ PI: Tresa Pollock (pollock@engineering.ucsb.edu); Author: Andrew Polonsky (polonsky@umail.ucsb.edu)

Additive manufacturing (AM) represents an economical and less labor-intensive process for on-demand production of advanced engineering components, and may also enable design of new hierarchically-structured materials. The integrity of AM parts has yet to be demonstrated for operations involving high temperatures, dynamic-loading, and/or radiation, hindering the application of this technology. This research, supported by the NNSA via the SSAA program over the last year, seeks to gain insight into the connection between processing parameters in AM techniques and the resulting distribution of microstructural features as compared to traditionally processed components. Such information is a critical element of a modeling infrastructure that will allow for the strategic development of engineering materials and stockpile-type components.

"A major challenge exists in that additive processes such as electron beam melting and laser engineered net shaping (LENS) inherently operate at the mesoscale, with molten pools on the order of millimeters in extent. Thus, high fidelity 3D information on material structure and defects at the millimeter-scale with nanometer resolution is critical," said Dr. Pollock.

The TriBeam, a novel diagnostic technique developed at the University of California, Santa Barbara, has been employed to provide microstructural and defect data over length scales relevant to additive processes. The TriBeam utilizes a femtosecond-laser (Ti-sapphire, 1.2-W average power, 1-kHz repetition rate, 780 nm, 120-fs pulse length[1]) and fast-steering mirrors for low-damage micromachining inside of a traditional scanning electron microscope equipped with a focused ion beam (FIB) and a full suite of characterization tools such as secondary electron and backscatter electron imaging, and electron backscatter diffraction (EBSD) and energy dispersive x-ray spectroscopy detectors. The system allows for the rapid generation of large three-dimensional (3D) datasets on the order of a cubic millimeter, with data acquisition rates more than four orders of magnitude faster than existing 3D tomography techniques such as serial sectioning via FIB or mechanical polishing. Utilization of the detector suite creates rich multi-modal datasets, acquired on timescales on the order of one to three days in fully-automated fashion. As the melt pools in AM are also on the order of a cubic millimeter, the TriBeam is uniquely equipped to probe these processes at the mesoscale.

Additively manufactured samples of stainless steel produced via a LENS process were characterized in their as-deposited state to observe the microstructure via traditional techniques. Large morphological differences were observed in transverse cross-sections as compared to longitudinal cross-sections, with transverse cross-sections exhibiting fan-like, semi-circular structures arising from adjacent melt pools, and longitudinal cross-sections exhibiting a "V"-shaped morphology characteristic of high-speed-welding processes. The strong dependence of microstructure on process necessitates the collection of 3D data in the TriBeam to identify representative volumes for construction of statistically-significant mechanical models of these additive samples.

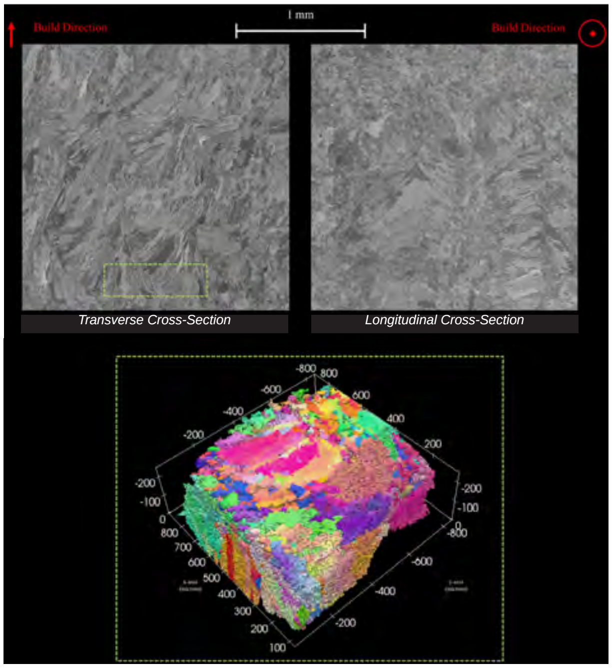

Figure 1. Cross-sections of 304L stainless produced via LENS, and a 3D reconstruction of TriBeam data. Grain orientations shown with inverse pole figure coloring.

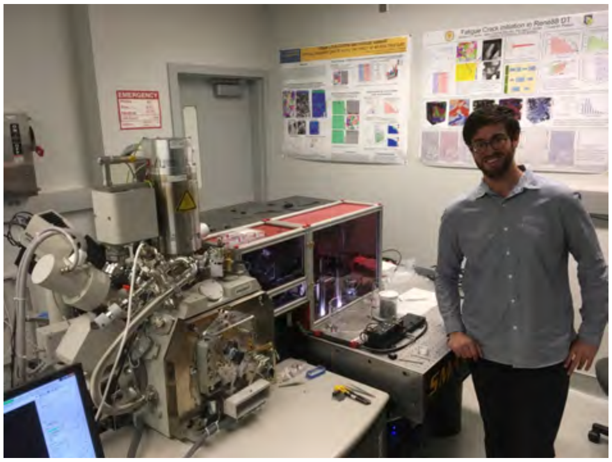

Figure 2. PhD student Andrew Polonsky with the TriBeam.

In an initial experiment, a volume of 800×800×250 microns was characterized in 60 hours in the TriBeam. Laser-based sectioning of each slice was followed by glancing-angle FIB to smooth the surface of laser-induced periodic surface structures and allow for clean EBSD patterns. Reconstruction was performed in the DREAM.3D framework to create coherent volumes from individual slices, and revealed the complex 3D shape of grains created in the LENS process. These results show the capability of the TriBeam to study additive processes and assess microstructural volume elements beyond traditional characterization techniques.

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Studying Extreme States of Matter with Pulsed Power Machines

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

Introduction

The scientific goal of the Center for Pulsed Power Driven High Energy Density Plasmas at Cornell University (the Center) is to achieve an understanding of the physics of current-driven high energy density plasmas. To accomplish this, we use 0.5-1 MA pulsed power machines to carry out experiments that are supported by computer simulations and theoretical modeling. Cornell has five research partners in the Center: the University of California, San Diego, Princeton University, Imperial College, the Weizmann Institute of Science (WIS), and the P. N. Lebedev Physical Institute. Together with the students, faculty, and staff at Cornell (see Figure 1), all of these partner groups contribute to the scientific output of the Center through experiments, theory, and diagnostic development, and to the education and training of students and postdoctoral researchers in the field of High Energy Density Laboratory Plasmas. During the contract year 2015-16, there were seven PhD graduate students at Cornell and five others at partner institutions supported fully or partially by Center funds, along with a total of four postdoctoral associates. The Center has been funded since October 2002, as part of the Stewardship Sciences Academic Programs. Since then, a total of 13 PhD students supported by Center funds at Cornell or Center partner institutions have become members of the scientific staff at NNSA's national laboratories. Some of our recent research accomplishments are described briefly in the following paragraphs.

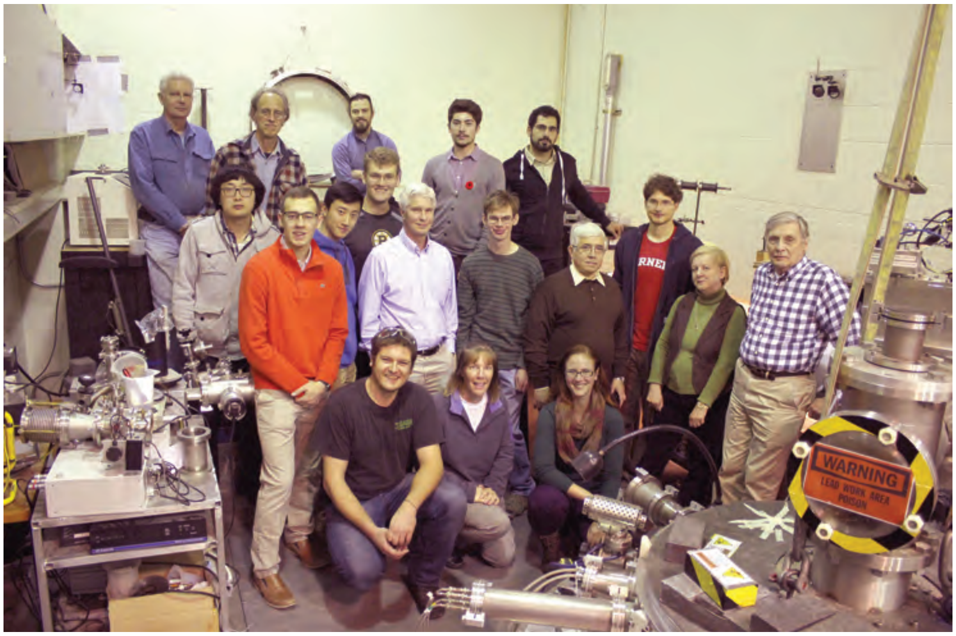

Figure 1. Cornell students, staff, and faculty of the Center for Pulsed Power High Energy Density Plasmas are pictured in the 1 MA COBRA pulsed power machine laboratory.

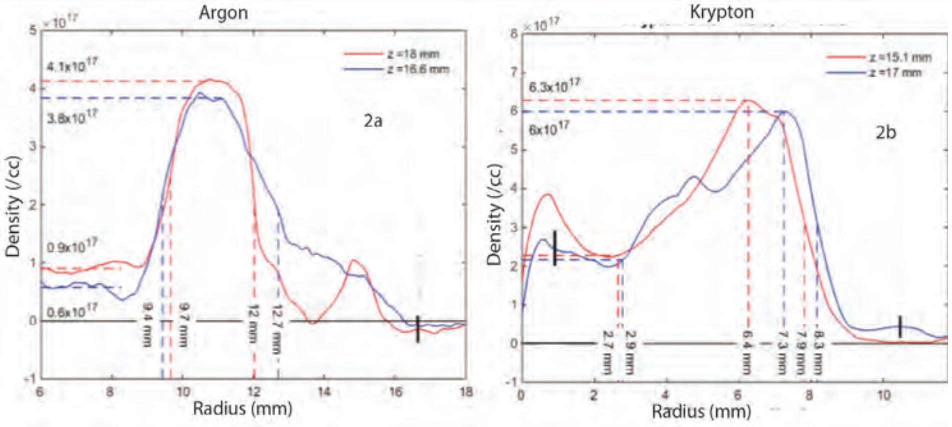

Figure 2. Radial profiles of argon and krypton shocks.

Gas Puff Z-Pinch

Studies of shock waves driven in gas puff Z-pinch experiments have been carried out on the 1 MA COBRA pulsed-power generator using a tri-axial gas puff valve that was developed together with our WIS colleagues. The gas is pre-ionized and then the 200-ns current pulse generates magnetic pressure on the outside of the plasma that acts like a piston to drive a shock in the plasma as the implosion develops. The interface between the magnetic field and the shocked plasma is unstable to the Magneto-Rayleigh-Taylor (MRT) instability and this instability can affect the implosion dynamics. Such experiments are used to generate x-ray pulses, and the MRT is found to adversely affect the efficiency of the x-rays generated when the implosion stagnates on the axis.

Radial density profiles obtained using a laser interferometer during the implosion are shown in Figure 2 where the shocked plasma is moving toward the axis on the left. Two types of shocks have been observed. With argon the shocked plasma density is fairly uniform, Figure 2a. With krypton the plasma density varies approximately linearly, Figure 2b. The unstable surface is at a radius of 12 mm (Figure 2a) and 8 mm (Figure 2b), respectively. The instability has been observed to have a higher growth rate for argon, in agreement with theoretical predictions.[1]

Laboratory Plasma Jets

Plasma jets formed from exploding foils in radial geometry have been studied with and without an applied magnetic

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field (B_z) parallel to the axis of the jet. Experimental results are compared with predictions made by an extended magnetohydrodynamics (XMHD) code, PERSEUS, that includes Hall and electron inertia terms in the generalized Ohms Law. Using COBRA in "standard polarity," the current (J) flows radially inward through a thin circular metal foil and down an axial cylindrical pin located beneath the foil. The current creates a surface plasma above the foil, and the J×B forces drive a plasma jet upward along the cylindrical axis. With an applied B_z of about 1 T, the plasma jet rotates azimuthally due to the J_rB_z component of the force and forms a conical plasma with density minimum on axis, as shown in Figure 3. Thomson scattering of 527-nm laser light shows azimuthal jet rotation of about 20 km/s. We determined that it is important to scale down the energy of the Thomson scattering laser to minimize its perturbation of the jet while still allowing the measurement.

The applied B_z was compressed by about a factor of 2 as the plasma converged to form the jet as measured using B-dot probes. Additionally, differences in the jet structure were observed depending upon whether the current flowed radially outward ("reverse polarity") or radially inward through the foil. There was more radial spread of the jet in reverse polarity. This change is predicted by the XMHD code but not by a pure MHD one because the low-density plasma dynamics, responsible for the formation of the higher density plasma jet, are more accurately handled with XMHD.[2]

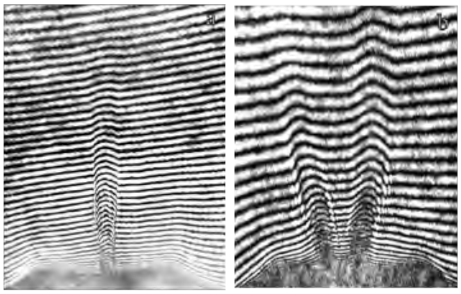

Figure 3. Laser interferometry of unmagnetized (a) and magnetized (b) plasma jets.

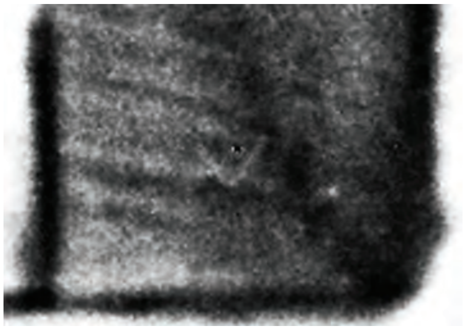

Figure 4. Extreme ultraviolet image of helical striations. The liner diameter is 8 mm.

Cylindrical Liners

Radiographic images of current-carrying metal cylinders, known as "liners," on the Sandia National Laboratories (SNL) Z machine have shown horizontal or helical structures depending on the absence or presence of an external axial magnetic field. Those features have been reproduced in extreme ultraviolet self-emission images (XUV)[3] using COBRA and 8-16 mm diameter, 1 cm long, 4 to 8-μm-thick Al liners, as shown in Figure 4. We have studied these ≈ 600-750 μm structures throughout the 200-ns current pulse. We have shown that applying a magnetic field changes the horizontal striations into left-handed or right-handed helical structures depending on the direction of the magnetic field. We believe these features are not due to Rayleigh-Taylor instabilities as our 1 MA current pulses do not implode the liner.

With high-resolution soft x-ray imaging, smaller scale (≈ 5-40 μm) discontinuous density variations perpendicular to the current flow were observed. Copper, titanium, and aluminum were tested and these features varied with material and the orientation of the current flow with respect to manufacturing defects.

The PERSEUS XMHD Code

The MHD model is expected to be valid for studying plasmas at the high densities and so it is commonly used for computational modeling of high energy density physics (HEDP) experiments. However, MHD fails to describe experimental results in many situations, most notably due to the omission of the Hall term in the Ohm's Law included in XMHD. We have investigated these failings by directly comparing MHD and XMHD simulations with HEDP experimental results to draw conclusions about the importance of the Hall term to obtaining agreement with the experiments. For example, for the MagLIF experiment on the Z machine at SNL, we find that ablation in the power feed leads to a low-density plasma in the region surrounding the liner. The inflow of this plasma compresses axial magnetic flux onto the liner. In MHD, this axial flux decays resistively, whereas in XMHD, a force-free current layer sustains the axial flux on the liner, leading to a larger ratio of axial to azimuthal flux than with MHD, and a compressed axial magnetic field as large as 1,000 T. During the liner compression, the MRT instability leads to helical perturbations consistent with experimental observations.

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Center of Excellence for Radioactive Ion Beam Studies for Stewardship Science

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

The Center of Excellence for Radioactive Ion Beam Studies for Stewardship Science (RIBSS), established in 2003, has been a leader in low-energy nuclear science and in attracting and training early career scientists. Rutgers University leads as the Center's consortium of scientists from the University of Tennessee-Knoxville, Michigan State University, Louisiana State University, University of Notre Dame, Tennessee Technological University, Oak Ridge National Laboratory (ORNL), and Lawrence Livermore National Laboratory (LLNL). The focus uses radioactive ion beams of fission fragments and other rare isotopes to study reactions on and structure and decay of atomic nuclei far from stability. These studies also help us understand the origin of the elements. These efforts require new theoretical approaches, new experimental tools, and a highly talented team that includes graduate students and postdoctoral scholars. In Fall 2016, 10 graduate students and 6 postdoctoral scholars are supported at least in part by the RIBSS Center. Three alumni of the Center are staff members at LLNL and two are postdoctoral researchers at LLNL and three at Los Alamos National Laboratory (LANL).

"The SSAA has given me the opportunity to introduce graduate students and postdoctoral scholars to a wide spectrum of fundamental and applied research opportunities in nuclear science at Livermore and Los Alamos National Laboratories, as well as enabling these early career scientists to engage in fundamental research at the frontiers of interdisciplinary research in nuclear astrophysics. Every year, I have had the privilege to host 15-20 students and postdocs at these NNSA laboratories and have been delighted when many of them have used these connections to join the laboratories as postdocs and the path to longer term careers," states Dr. Jolie Cizewski, the Principal Investigator (PI) of the Center.

Research Highlight: Nuclear Reaction Studies at the National Superconducting Cyclotron Laboratory

One of the challenges in nuclear physics is to identify regular patterns in the structure of heavy atomic nuclei and use these patterns to help us to understand the nature of the nuclear force. The RIBSS Center has been using the tools developed under the SSAA for nuclear reaction and beta decay experiments to measure detailed spectroscopy of nuclei away from stability. This experimental effort has also required a close coupling with advances in nuclear reaction theory of weakly bound nuclei.

The RIBSS Center has been a leader in using the neutron transfer (d,p) reaction to measure the single-neutron character of excitations in nuclei near the closed shell of 50 neutrons and the weak r-process path of nucleosynthesis. The development of the Oak Ridge Rutgers University Barrel Array (ORRUBA)[1] has enabled detailed measurements of reaction cross sections as a function of angle, measurements that are critical to deducing properties of the final states when compared with the expectations from theoretical reaction calculations. In addition to developing new experimental tools, this effort has also required state-of-the art-theoretical modeling of the (d,p) reaction, since the deuteron is weakly bound (e.g., reference 2).

At many accelerator facilities, the beam energies are not significantly higher than the energy necessary to overcome the Coulomb repulsion of the positively charged beam and the deuterons in the targets. At these low energies, the measured reaction cross-sections probe only the tail of the wave function, rather than the nuclear interior. However, the National Superconducting Cyclotron Laboratory (NSCL) can accelerate stable and unstable beams to more than an order of magnitude higher energies, with the potential to probe more of the interior of the nucleus and, hence, details of the nuclear wave functions. To capitalize on the opportunities at NSCL, the Center and its collaborators have developed a new capability to measure (d,p) reactions with ORRUBA and fast beams.

The proof-of-principle measurements were made in Winter 2014 when ORRUBA was mounted in front of the S800 magnetic spectrograph at NSCL. A total of 3,000-MeV (35 MeV/u) beams of stable ^{86}Kr interacted with CD_2 targets at the center of the ORRUBA chamber. Light reaction protons were detected with the ORRUBA barrel, supplemented by the Silicon Detector Array (SIDAR)[3] at back angles. Rutgers PhD student David Walter, shown in Figure 1, has been leading the analysis of these data, working closely with RIBSS Center co-PI Professor Filomena Nunes in using state-of-the art reaction theory to interpret the results. Nunes and her colleagues[4] had proposed that a better measure of the radius and diffuseness of the nuclear potential could be deduced by combining the results from a relatively low-energy study, to characterize the tail of the wave function, with a higher energy measurement, that probes further into the nuclear interior. The interpretation of the ^{86}Kr(d,p) reaction included analysis of cross sections from an earlier measurement[5] at much lower energies.

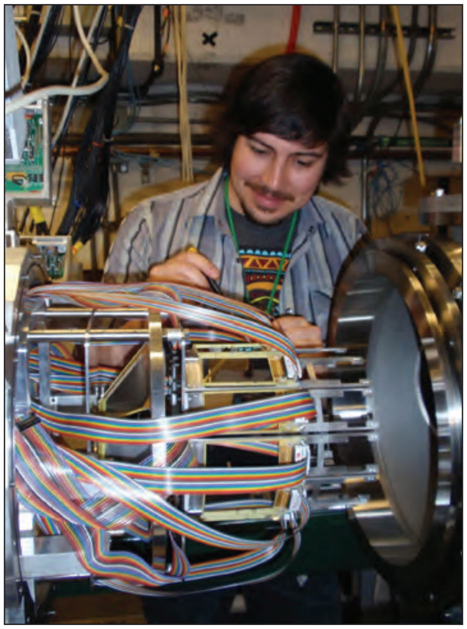

Figure 1. Rutgers PhD student David Walter with the ORRUBA and SIDAR charged-particle detector setup at the NSCL in Winter 2014.

Preliminary results from combining the low (predominantly peripheral) and higher (less peripheral) energy measurements are displayed in Figure 2. The spectroscopic factor *S* informs the fragmentation of the single-neutron strength; *S*=1 means a pure single-particle configuration, *S*<1 means that the strength is fragmented over more than one state. *S* is deduced

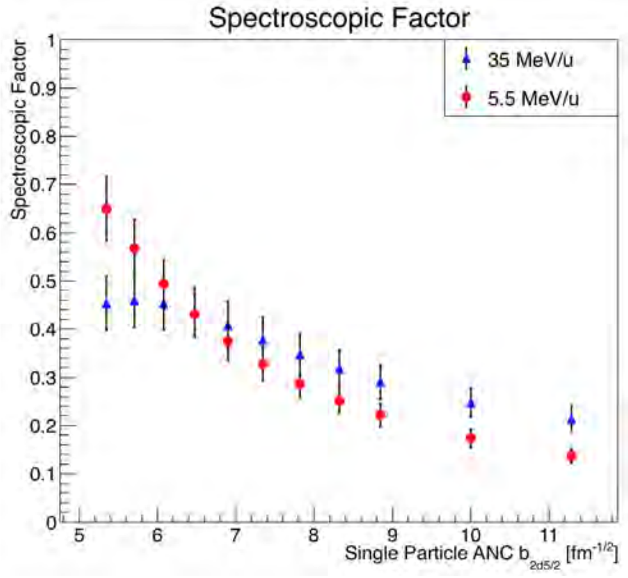

*Figure 2. Spectroscopic factors for the 2d$_{5/2}$ ground state of ^{87}Kr as a function of the single-particle ANC deduced from 5.5 MeV*A data (red circles)[4] and 35 MeV*A data (blue triangles).[5]*

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by comparing experimental differential cross sections to theoretical ones. The theoretical calculations make assumptions for the mean field potential in which the transferred neutron is bound; these assumptions produce different single-particle asymptotic normalization coefficients (spANC), *b*. Since we do not know the exact form of the mean field, this introduces an ambiguity in the problem that can be greatly reduced if two measurements are performed, one at low energy, where the reaction is peripheral, and the other at higher energy.

For a low-energy, peripheral, reaction *S* is expected to vary significantly as a function of the spANC, as is observed in Figure 2 for the spectroscopic factor for the ground state in ^{87}Kr deduced from the low-energy data. At a higher energy, the dependence on *S* as a function of spANC is expected to be flatter, as is observed for the spectroscopic factor for the ground state in ^{87}Kr deduced from the NSCL data. Since *S* characterizes the properties of a particular level, independent of the beam energy, we find that $S\approx0.4$ is consistent with both measurements, corresponding to a nuclear radius $R\approx6$ fm and diffuseness somewhat larger than values usually assumed.

The success of combining a low and higher energy measurement to constrain spectroscopic properties supported the approval by the NSCL management of the next measurement with ORRUBA and radioactive ^{84}Se beams that are near the weak r-process path of nucleosynthesis.

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Studies in Low Energy Nuclear Science

Ohio University ❖ PI: C.R. Brune (brune@ohio.edu); Authors: A.V. Voinov (voinov@ohio.edu), C.R. Brune, S.M. Grimes, and T.N. Massey

In addition to fundamental applications in physics and astrophysics, low-energy nuclear reactions play a vital role in many aspects of our life, including nuclear technology and national security. The low-energy nuclear studies at the Edwards Accelerator Laboratory focus on measurements of reaction cross sections, the study of nuclear structure properties that govern these cross sections, improving the predictability of models, and the development of experimental techniques. Much of the research is centered around producing and detecting neutrons. The bulk of these studies are carried out by graduate students, and the training of students is also a focus of our program. Two of our graduate students are currently supported by the SSAA Program.

Figure 1. Ohio University faculty members C.R. Brune and A.V. Voinov (in the center) with graduate students (from left to right): S.N. Paneru, S. Dhakal, C.E. Parker, and A.L. Richard at the 2016 SSAP Symposium.

Students obtain hands-on experience working with detectors and electronics, operating our local tandem accelerator, and performing computer data analysis and simulations. They participate in scientific projects starting from developing the ideas to the final publications in scientific journals. In addition, some of our experiments are done at other laboratories and our students have the opportunity to gain this additional experience.

Low-energy nuclear reactions, where energy of projectiles are up to 5 MeV/A, are the type of reactions important for the nuclear power industry and national security. The experimental study of nuclear structure properties such as the nuclear level density, the γ-strength function, and optical model potentials is an important direction of experimental research conducted at the laboratory. These quantities are used as an input for calculation of reaction cross sections, including reactions with neutrons important for nuclear power and r-process nucleosynthesis. A new computer code based on the statistical Hauser-Feshbach model has been developed, including novel features such as isospin conservation (complete or partial), the calculation of the angular distribution of reaction products, and the effect of nuclear deformation.

The nuclear level density is studied experimentally with charged-particle induced reactions creating compound nuclei which "evaporate" particles similar to how boiling water evaporates molecules. It turns out that spectra of evaporated particles and molecules are very comparable, indicating a similarity of these two processes. These spectra are primarily determined by the density of final states. The γ-strength and optical potentials determine probability of emission of γ-rays and particles from excited states of nuclei, as well as the inverse processes, i.e., the probability of fusion. They are studied with experiments producing γ-rays from nuclear reactions and with elastic scattering of particles on nuclei, respectively. The observed enhancement is a new feature of the γ-strength function at low (E_γ<3 MeV) energies that is a topic of increasing interest. It is addressed in our laboratory by the measurements of cascade γ-transitions from low-energy proton capture reactions.

Cross section studies of specific reactions of interest for applications are conducted. One of these is for neutron transport in iron and is performed using an iron sphere surrounding a pulsed neutron source generated by our accelerator beam. This technique allows one to test elastic and inelastic cross sections which are considered to be much more uncertain compared to the total neutron cross section. Other ongoing projects involving specific reactions include ^{3}H(d,γ) and ^{13}C(n,Xγ). Accurate knowledge of these and some other reactions is important for diagnostics of laser-induced inertial confinement fusion at the National Ignition Facility (NIF) located at Lawrence Livermore National Laboratory (LLNL) and the University of Rochester Laboratory for Laser Energetics. One of our PhD graduates, Daniel Sayre, is on the research staff at LLNL working on NIF diagnostics. Neutron-induced reactions on ^{10}B are poorly known for neutron energies above a few hundred keV. We have performed such measurements using Los Alamos National Laboratory's WNR/LANSCE facility where proton, triton, and α-particle exit channels were detected.

Our laboratory is well equipped with different kinds of charged-particle and γ-ray spectrometers. The unique 30-m underground tunnel coupled to a beam swinger allows precise measurement of reactions with neutrons using the time-of-flight technique. The laboratory is an attractive place for other researchers to come and conduct experiments and they are always welcome. More information can be found at http://inpp.ohiou.edu/~oual.

Microscopic Description of the Fission Process

Michigan State University ❖ PI: W. Nazarewicz (witek@frib.msu.edu)

Our understanding of nuclear fission, a fundamental nuclear decay, is still incomplete due to the complexity of the process. Since 2003, we have carried out a study of the nuclear fission process supported by the SSAA Program. Our principal goal is to obtain a comprehensive understanding of the nuclear fission process by taking advantage of state-of-the-art theoretical techniques and advanced computational resources. The current grant supports two graduate students and a postdoctoral associate. One of our former postdoctoral scholars works at Lawrence Livermore National Laboratory as a research staff.

The SSAA grant has enabled us to launch programmatic research on the theory of nuclear fission, which requires a serious long-term commitment. Thanks to conceptual and algorithmic developments achieved, a coherent microscopic nuclear fission theory, based on quantified input, is on the horizon. Training of next-generation nuclear theorists is an essential part of our undertaking, and Figure 1 shows two graduate students involved. During the course of the grant, several graduate students were involved in our fission research. All of them participated, and exhibited, in the annual Stewardship Science Academic Programs Review Symposia, and were exposed to the broad NNSA research agenda.

Large-scale simulations of the fission process are crucial for many areas of science and technology. Fission governs the existence of many transuranium elements, including the predicted long-lived superheavy species. In nuclear astrophysics, fission influences the formation of heavy elements on the final stages of the r-process in a very high neutron dense environment. Fission applications are numerous. Improved understanding of the fission process will enable scientists to enhance the safety and reliability of the Nation's nuclear stockpile and nuclear reactors. The deployment of a fleet of safe and efficient advanced reactors, which will also minimize radiotoxic waste and be proliferation-resistant, is a goal for the advanced nuclear fuel cycles program. While in the past the design, construction, and operation of reactors were supported through empirical trials, this new phase in nuclear energy production is expected to heavily rely on advanced modeling and simulation capabilities.

Figure 1. Two graduate MSU students supported by this SSAA grant, Zachary Matheson and Chunli Zhang, analyze computed fission pathways.

Under this SSAA project, we study the phenomenon of spontaneous fission using the symmetry-unrestricted nuclear density functional theory. Our results show that many observed properties of fissioning nuclei, such as half-lives and yield distributions, can be explained in terms of pathways corresponding to different geometries of fission products. Our calculations demonstrate that properties of fission vary rapidly with particle number. Not only does this reveal clues about the conditions for creating new elements, it also provides a wider context for understanding other types of fission. Recently, we developed a methodology to calculate mass and charge distributions of spontaneous fission yields using advanced simulations. The method combines the multi-dimensional minimization of collective action for fission with stochastic Langevin dynamics to track the relevant fission paths from the ground-state configuration up to scission. As seen in Figure 2, we obtained a quantitative agreement with experimental data for both the charge and mass distributions in the spontaneous fission of ^{240}Pu.

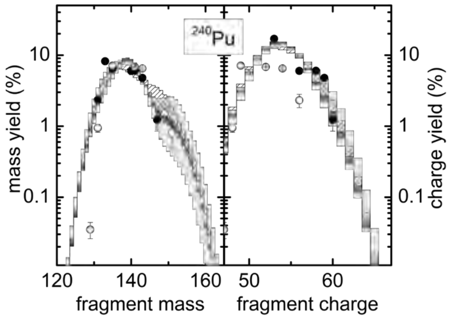

Figure 2. Predicted mass and charge distributions of spontaneous fission yields of ^{240}Pu compared to experiment (circles). The shaded regions are uncertainties in the computed distributions due to variations of model parameters. From Sadhukhan, Nazarewicz, and Schunck, Phys. Rev. C 93, 011304(R), 2016.

The principal impact is in the delivery of high-fidelity fission models capable of providing nuclear data not only of a higher quality, but also with quantified uncertainties. For many NNSA applications, the required data on fission cross sections or fission products cannot be obtained via experiment, because very neutron-rich nuclei with short half-lives are required. Simulating fission, and in particular modeling properties of fission fragments, is essential to successfully analyzing fission yields under a variety of conditions.

Determination of Thermodynamic and Kinetic Parameters for Complexation of Tc(IV)

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A thorough understanding of the chemistry of fission products is key for better and earlier detection of these fission products for nuclear forensics purposes. In particular, technetium ^{99}Tc represents an important radionuclide, because it is produced in high yield (6% of the fission products) upon ^{235}U or ^{239}Pu fission. The chemistry of Tc(VII) as the pertechnetate anion TcO_4 is well understood, but critical gaps remain in the understanding of the chemical behavior of Tc(IV), which occurs under mildly reducing conditions. The goal of this research is to determine thermodynamic and kinetic parameters for the complexation of Tc(IV) with the halides, sulfate, phosphate, carboxylate ligands (e.g., acetate, citrate, oxalate), and aminocarboxylates (e.g., ethylenediaminetetraacetic acid [EDTA]). In particular, stability constants (and Gibbs free energies, ΔG), enthalpies (ΔH), and entropies (ΔS) will provide essential data to develop understanding and predictive capability of Tc(IV) aqueous solution behavior. This is our first project supported by the SSAP. The work is carried out by Cecilia Eiroa-Lledo, a graduate student who has recently become a U.S. Nuclear Regulatory Commission-licensed nuclear reactor operator for the Washington State University (WSU) TRIGA reactor (thanks to this program), and Gannon Parker, a postdoctoral research assistant.

“This grant program provides a valuable opportunity for developing excellent science, while training students in the field of nuclear sciences,” Principle Investigator Nathalie A. Wall said.

Gannon Parker choses to use metastable ^{99m}Tc to carry out ultra-low level tracer experiments (< 10^{-9} M). He can generate ^{99m}Tc onsite, using the WSU research reactor, by irradiating stable ^{98}Mo with neutrons and loading the resulting ^{99}Mo onto an alumina column to produce a ^{99m}Tc generator (see Figure 1). He produces a new generator every two weeks, due to the short half-life of ^{99}Mo ($t_{1/2}$ = 66 hours). Experiments carried out with ^{99}Tc (obtained from Oak Ridge National Laboratory) allow Gannon to perform experiments at higher concentration (~10^{-7} M). He determines stability constants (and ΔG) for the complexation of Tc(IV) using a liquid-liquid extraction (LLE) method over a wide range of ionic strengths. LLE conducted over a range of temperatures allow for the determination of ΔH and ΔS. Gannon can also identify the extractable Tc(IV) species from LLE data in absence of ligand, from the distribution coefficient of Tc (D, the ratio between Tc concentration in the organic phase and that in the aqueous phase) as a function of the concentration of the extractant or as a function of pH (see Figure 2). Cecilia Eiroa-Lledo is currently determining accurate Pitzer parameter coefficients, because they are necessary to build accurate models for the prediction of Tc chemical behavior in solutions in a wide range of ionic strengths and compositions. Pitzer parameters of common salts and metals have been reported extensively in the literature for some of the compounds of interest, but Cecilia found significant differences among the reported values. This research provides an experimental comparison of parameters found using LLE and those found using the change in the molal volume of the solution being studied. This suite of experiments is critical in building a predictive model for Tc(IV) complexation in environmental systems.

Figure 1. ^{99}Mo is loaded onto the column and ^{99m}Tc may be eluted from the column as the ^{99}Mo decays.

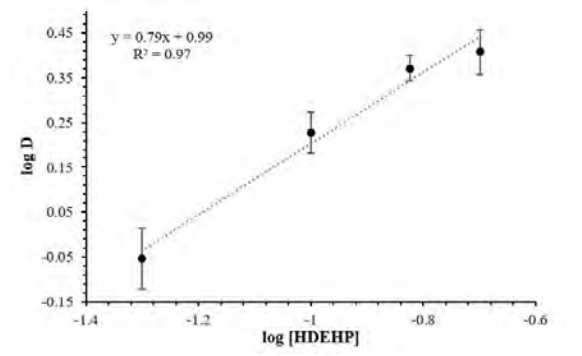

Figure 2. Representative plot of the distribution ratio between the aqueous and organic phases of the LLE experiment as a function of the concentration of the extractant ([HDEHP]). The slope of 0.8 ± 0.2 indicates that the species being extracted is the monovalent TcO(OH)+ ion.

Richard Hughes, Lawrence Livermore National Laboratory (hughes61@llnl.gov)

Years at LLNL: 07/2013-Present ❖ Degree: PhD, Nuclear Physics ❖ SSAP Program: 2010-2013, University of Richmond

After obtaining my doctorate in experimental nuclear physics, I moved to Richmond, Virginia to begin a postdoctoral position at the University of Richmond (UR) working with Professor Cornelius Beausang. When I arrived in Richmond, I was relatively unfamiliar with stockpile stewardship research and its importance in ensuring the safety and security of the Nation.

During my appointment at UR, support from the SSAA program enabled me to apply my nuclear physics background to measurements of cross sections for neutron-induced reactions (such as n-gamma and n-fission) in unstable nuclei that are relevant to stockpile stewardship applications. Cross sections of very short-lived nuclei (<100 days), are difficult or even impossible to measure directly and, in order to deduce these cross sections, surrogate reactions employing accelerated beams of light ions to bombard targets can instead be used to simulate the neutron-induced reaction. The cross sections of interest are subsequently deduced from the experimental data with theoretical corrections to account for differences in the neutron and surrogate reactions.

Over the course of my time at UR, our group, in collaboration with scientists from Lawrence Livermore National Laboratory (LLNL) and other institutions, conducted several surrogate reaction experiments to measure n-fission cross sections in actinide nuclei, in addition to basic science experiments. The measurements utilized the STARLiTeR detector array that combined a silicon telescope for measuring light ions/fission fragments and up to six high-purity germanium (HPGe) detectors for simultaneous detection of gamma rays. The experiments were conducted at both Lawrence Berkeley National Laboratory (LBNL) and Texas A&M University (TAMU), and during the periods I spent at these institutions, I acquired experimental skills and techniques that have been important to my development as a scientist. It was also during these periods that, while talking to my LLNL collaborators, I learned more about the NNSA national laboratories and decided that a career performing research addressing the needs of the Nation's security, specifically at a national laboratory, appealed strongly to me.

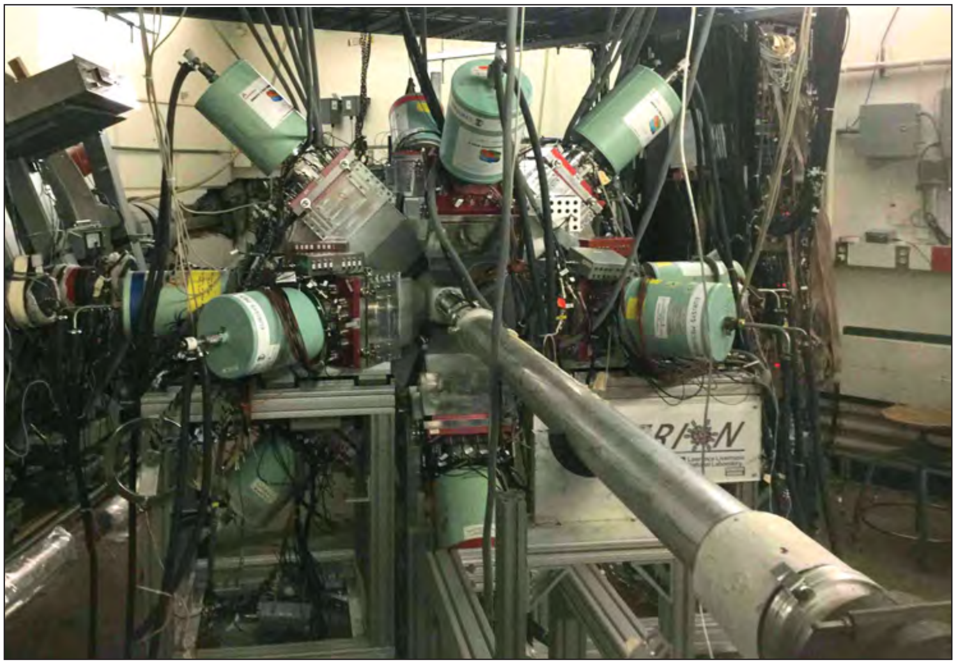

Figure 1. The NNSA-funded Hyperion array consists of a silicon telescope for detecting ions and fission fragments and a surrounding array of up to 14 HPGe detectors for simultaneously measuring gamma rays. Hyperion is housed at Texas A&M University Cyclotron Institute where it is used for stockpile stewardship and basic science experiments.

In July 2013, shortly after presenting the UR research summary at the SSAP annual symposium, I moved to Livermore, California, to begin a postdoctoral position at LLNL. I worked with Dr. Robert Casperson and Dr. Jason Burke on several projects focusing on both basic science and stockpile stewardship studies. During the second year of my postdoctoral position, I was tasked with replacing the STARLiTeR array with the new Hyperion array. The upgrade, which would increase the maximum capacity of HPGe detectors from six to fourteen, was essential for improving surrogate measurements of n-gamma cross sections. Hyperion was designed, constructed, and assembled over the course of a year and its commissioning experiment was performed in August 2015. The array is situated in cave 4 of the TAMU Cyclotron Institute and is shown in Figure 1.

In June 2016, I accepted a staff scientist position at LLNL. I continue to work on research focused on stockpile stewardship and basic science in nuclear physics, in addition to projects with applications in homeland security. The support provided by the SSAA during my postdoctoral research afforded me the opportunity to collaborate closely with scientists from different national laboratories and to become involved in stockpile stewardship research. The SSAA program was thus instrumental in guiding my career path, which has led to my present position at LLNL.

Patricia Kalita, Sandia National Laboratories (pekalit@sandia.gov)

Years at SNL: 2015 -Present ❖ Degree: PhD, Physics ❖ SSAA Program: 2008-2015, University of Nevada, Las Vegas

My introduction to the SSAP was as an undergraduate at the University of Nevada Las Vegas (UNLV), where I joined Professor Andrew Cornelius's group at the High Pressure Science and Engineering Center (HiPSEC). Continuing with an MSc and a PhD, I had the opportunity to learn about static high pressure physics and became a frequent user of the High Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source (APS) at Argonne National Laboratory (ANL). I was impressed by the dynamic atmosphere and always evolving research capabilities of HPCAT so with the support of the SSAP HiPSEC graduate program, I wrote a PhD project proposal that took advantage of the high pressure physics research capabilities at both the APS and at UNLV.

During my PhD work, I had the opportunity to meet a number of scientists from the NNSA national laboratories. At that time, I did not know what my career path would be and I certainly did not anticipate that choices I made in graduate school would lead me toward a position working at a national security laboratory.

My PhD project was a comprehensive investigation of the high-pressure structural behavior of several different mullites and synthetic mullite-type complex ceramic oxides. The materials were investigated at extreme pressures in diamond anvil cells, using synchrotron x-ray diffraction (at HPCAT) and laser Raman spectroscopy (at UNLV). These experimental techniques are ideally suited to providing a synergical interplay in the study of oxides under high-pressure conditions: Raman spectroscopy is a technique for investigating short-range-order phenomena, while x-ray diffraction accesses structural changes occurring at the long range order. My PhD work at HiPSEC led to a variety of findings in mullite-type materials: phase transitions, equations of state, pressure-driven amorphization, and the discovery of the very rare phenomenon of negative linear compressibility in some of the materials.

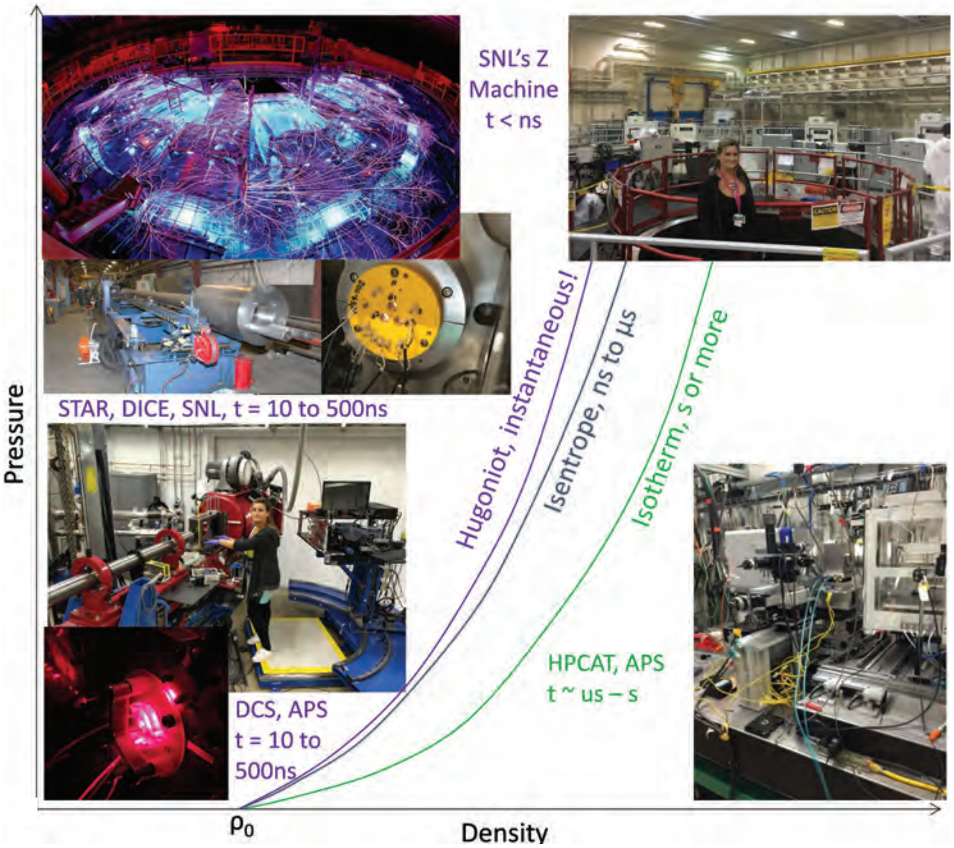

Figure 1. Cross-platform experimental effort to ascertain the influence of timescales on phase transitions in materials.

After graduating with my PhD in physics in 2015, I accepted a postdoctoral researcher position at Sandia National Laboratories (SNL) where I am now a member of the Dynamic Materials Department. My work focuses on materials' response to dynamic and static compression. I conduct experiments using SNL's Z machine, STAR, and DICE. I also lead SNL's effort at the Dynamic Compression Sector (DCS) at the APS, where I combine *in situ* x-ray diffraction with static compression. I also continue experimental work at HPCAT, combining x-ray diffraction with both static and ramp-compression. I am learning the importance of the work we do at national laboratories and how, through my research, I can explore fascinating phenomena while also contributing to the bigger picture. Access to world-class facilities allows me to work on cutting-edge shock physics research.

I am now working on a cross-platform experimental effort to ascertain the influence of timescales on phase transitions in materials. This effort, characterized in the figure, includes pulsed power dynamic material property experiments at the Z machine of SNL, impact experiments using a two-stage light gas gun at SNL, x-ray diffraction and impact experiments using a two-stage light gas gun at DCS, and ramp compression as well as static compression combined with x-ray diffraction at HPCAT. This combination allows me to explore shock and pressure-driven phenomena at the microstructural level and at different time scales. These experiments and cross-platform comparisons open the door to a new, unprecedented understanding of equations of state and of phase transitions, and will ultimately improve our capability to accurately simulate the behavior of materials at extreme conditions.

Nicholas Ouart, Naval Research Laboratory (nicholas.ouart@nrl.navy.mil)

Years at NRL: 2011-Present ❖ Degree: PhD, Physics ❖ SSAA Program: 1999-2010, University of Nevada, Reno

I was very fortunate to have been supported by the SSAA program in both my undergraduate and graduate studies at the University of Nevada, Reno (UNR). My faculty advisor was Professor Alla Safronova and my PhD dissertation was titled "Radiative Properties of Z-pinch and Laser Produced Plasmas from Mid-Atomic Number Materials." This research emphasized the diagnostic utility of x-ray spectroscopy on the emission from high energy density plasmas using non-local thermodynamic equilibrium kinetic modeling. Much of the experimental data that was modeled originated from two university pulsed power generators: Zebra at UNR and COBRA at Cornell University. The loads imploded were from many different z-pinch configurations and wire materials. During my university studies, I was always encouraged to present my results at scientific conferences and interact with many excellent scientists in the community.

After graduation, I started my postdoctoral work with a National Research Council Associateship Award at the Naval Research Laboratory (NRL) with Dr. John Giuliani as my advisor and was converted to a laboratory employee less than two years later. I pursued my career path with the Radiation Hydrodynamics Branch in the Plasma Physics Division at NRL because of their scientific expertise in coupling the atomic physics and the non-local radiation transport with the plasma dynamics to simulate and develop plasma radiation sources. The Branch collaborates with DOE/NNSA-supported scientists in support of the science-based Stockpile Stewardship Program.

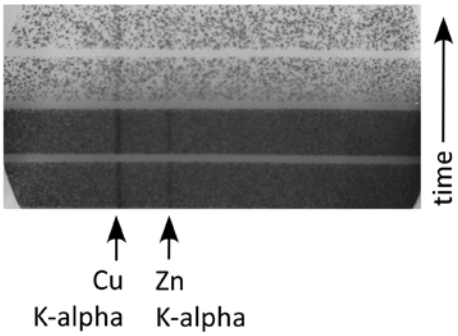

Figure 1. Time-gated K-shell spectra from the implosion of a compact cylindrical brass wire array using the Zebra generator with the Load Current Multiplier.

Wire array z-pinch plasmas on the Z machine at Sandia National Laboratories (SNL) have produced some of the most powerful x-ray sources using materials from aluminum to krypton. These x-rays are emitted as line radiation from highly charged ions stripped to the K-shell. There is interest in developing higher photon energy sources, but the energy required to ionize to the K-shell and the radiative losses from lower ionization stages is larger from higher atomic number materials. In pursuit of alternative mechanisms to provide the higher energy photons, we studied the Kα emission and L-shell radiation from brass wire arrays on the Zebra generator. In these experiments, the L-shell radiation comes from ionization stages around the Ne-like charge state that is largely populated by the thermal electron energy distribution function, while the K-shell photons are the result of high-energy electrons ionizing the inner-shell n=1 electron from ionization stages around the Ne-like ionization stage. An example of the time-gated measurements of the copper and zinc Kα lines is shown in Figure 1. We found that a simple runaway model for the energetic electrons could not account for the observed Kα yield.[1] In our collaboration, we also worked with SNL scientists to explore the Kα emission on the Z machine. It was found that the non-thermal emission had more favorable scaling and was more dominant than the thermal emission for atomic number materials over 42.[2]

Recently we have been collaborating with Lawrence Livermore National Laboratory to develop diagnostics using x-ray spectroscopy to infer the electron temperature in indirect drive inertial confinement fusion implosions on the National Ignition Facility (NIF). The electron temperature may be a better measure of the thermal hot spot compared to the ion temperature inferred from neutron spectral measurements. This is because the ion temperature is sensitive to the non-thermal velocity distributions in the fuel, whereas the electrons should not be sensitive to these bulk motions. A series of experiments has already been accomplished on NIF using krypton-doped capsule implosions.[3]

"I pursued my career path with the Radiation Hydrodynamics Branch in the Plasma Physics Division at NRL because of their scientific expertise in coupling the atomic physics and the non-local radiation transport with the plasma dynamics to simulate and develop plasma radiation sources. The Branch collaborates with DOE/NNSA-supported scientists in support of the science-based Stockpile Stewardship Program."

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These scientific endeavors have diversified my knowledge of radiation from high energy density plasmas. Working at the NRL and collaborating with DOE/NNSA-supported scientists has been an exceptionally rewarding experience, and I am very grateful to the Stewardship Science Academic Programs for the opportunities it has provided.

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“... CDAC has as its mission to expand the understanding of materials behavior at extreme pressure-temperature (P-T) conditions, develop new facilities and methods to advance high P-T materials research, and support the education and training of graduate students for work in areas of importance to Stockpile Stewardship.”

* * *

“The Center of Excellence for Radioactive Ion Beam Studies for Stewardship Science (RIBSS), established in 2003, has been a leader in low-energy nuclear science and in attracting and training early career scientists. Rutgers University leads as the Center’s consortium of scientists from the University of Tennessee-Knoxville, Michigan State University, Louisiana State University, University of Notre Dame, Tennessee Technological University, Oak Ridge National Laboratory (ORNL), and Lawrence Livermore National Laboratory (LLNL). The focus uses radioactive ion beams of fission fragments and other rare isotopes to study reactions on and structure and decay of atomic nuclei far from stability. These studies also help us understand the origin of the elements.”

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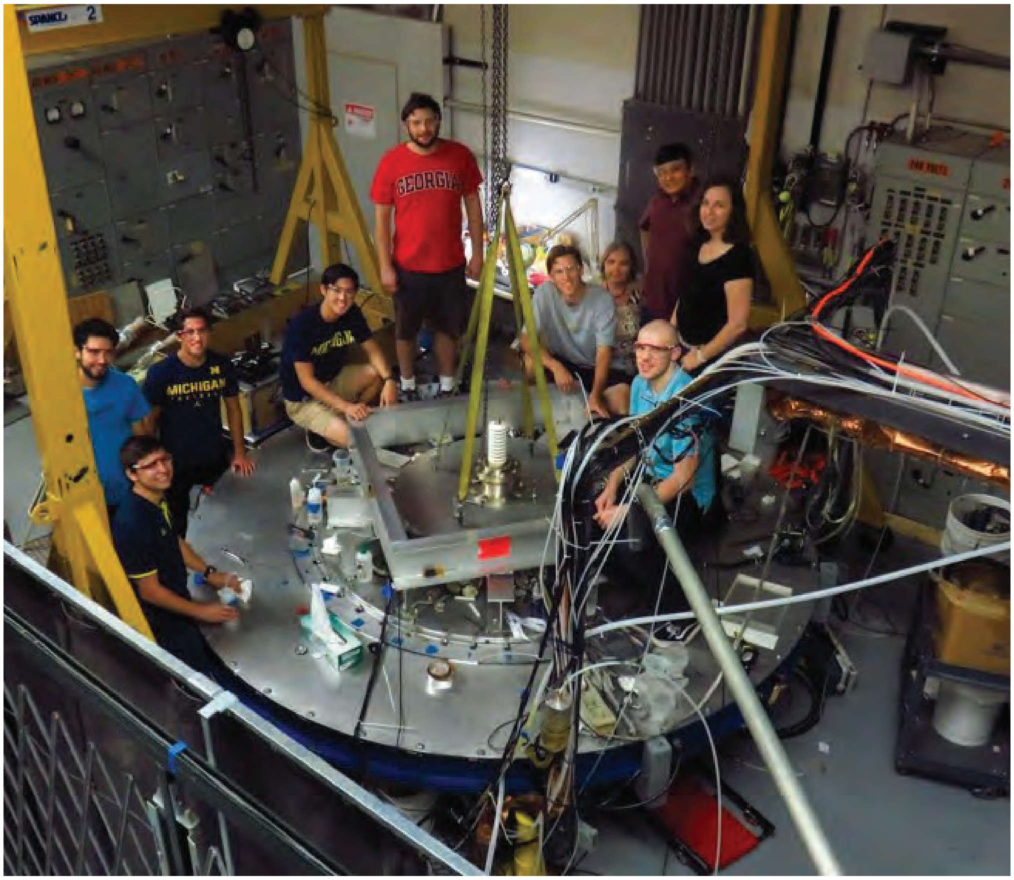

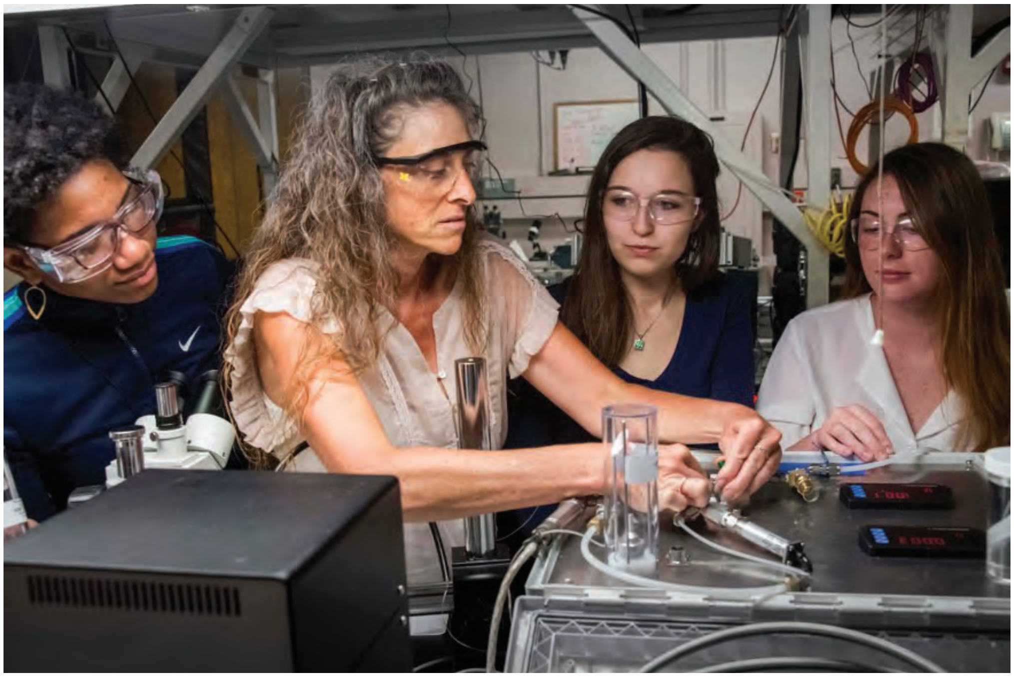

High Energy Density Laboratory Plasmas

Development of a Broadband Directional X-ray Source Platform for Radiography of HED Targets

University of California, Los Angeles ❖ PI: Chan Joshi (cjoshi@ucla.edu)

This project is concerned with developing a new diagnostic for probing matter under extreme conditions. The University of California, Los Angeles (UCLA) group led by Professor Chan Joshi is working on developing a directional broadband (40-80 keV) x-ray source base on periodic oscillations of electrons produced in a plasma accelerator driven by a picosecond laser pulse. The work is currently undertaken at the Jupiter Laser Facility in collaboration with Félicie Albert's group at Lawrence Livermore National Laboratory (LLNL) with the goal of fielding an experiment at the National Ignition Facility (NIF). The work, in its second year, has already produced significant results that have been submitted for publication.

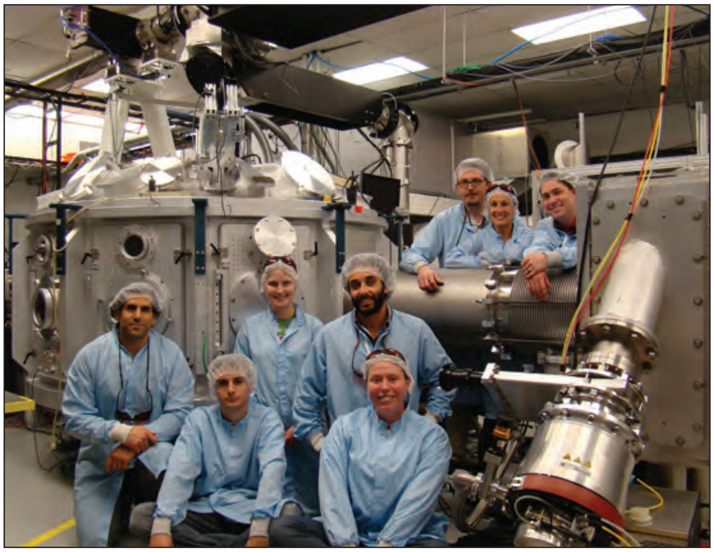

Figure 1. Experimental team at the Titan Laser Facility.

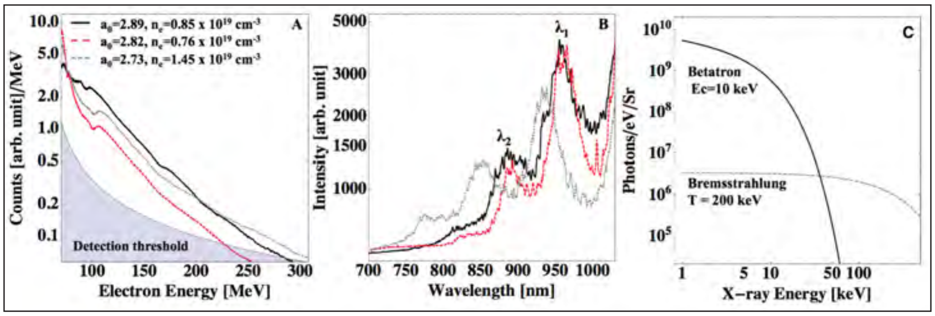

Figure 2. (a) Electron spectra for three different shots, (b) corresponding laser forward spectra showing the RFS satellites characteristic of the SM-LWFA regime, (c) Inferred betatron spectra and background Bremsstrahlung spectra (from electrons interacting with the chamber walls).

One student, Jessica Shaw, has graduated and gone to the University of Rochester Laboratory for Laser Energetics (LLE), and the postdoctoral scholar, Dr. Nuno Lemos, has taken up a similar position at LLNL. Dr. Lemos will continue to work on this project.

The development of directional, low-divergence, and short-duration (ps and sub-ps) x-ray beams with energies larger than 50 keV is of extreme importance to various fields of physics, e.g., high energy density (HED) science and inertial confinement fusion (ICF). They use the ps-pulse duration, kJ-class lasers, present in the majority of the HED facilities, to generate an x-ray source through betatron motion of the electrons in a Self-Modulated Laser Wakefield Accelerator (SMLWFA). Due to its directionality, relatively small divergence angle, high-brightness and high energy, this x-ray source overcomes the limitations of the conventional sources and can be an ideal probe and backlighter to support large-scale facilities such as OMEGA EP, LMJ-PETAL, and NIF-Advanced Radiographic Capability.

When a high-intensity (> 1×10^{18} W/cm^2) laser pulse with a pulse duration larger than the plasma period propagates through an underdense plasma, it can generate plasma waves through the Raman forward scattering (RFS) and self modulation (SM) instabilities of the laser pulse.[1] The experimental evidence for SM and RFS instabilities is the generation of sideband frequencies, which arise as a result of energy and momentum conservation. These plasma waves have an associated longitudinal and transverse field. The longitudinal electric field accelerates the self-trapped electrons to relativistic energies and the transverse field leads to betatron-like oscillations of the off-axis electrons, which then radiate photons in the forward direction and generate an x-ray beam. Furthermore, since the laser pulse will naturally overlap many plasma wavelengths, and therefore the accelerating electrons, there is a significant contribution from direct laser acceleration to the energy gained by the electrons[2] that further increases the x-ray energies.

At Titan (see Figure 1), for electron densities of 10^{19} cm^{-3} and laser intensities around 10^{19} W/cm^2, the acceleration of electrons up to 300 MeV (see Figure 2a) was observed. The measured laser spectrum in the forward direction (shown in Figure 2b) shows the presence of a series of satellites separated in frequency by the plasma frequency confirming that we are in the SMLWFA regime. As explained above, these electrons execute betatron motion as they are accelerated, and radiate in the x-ray region. The measured x-ray spectrum could be fitted with a synchrotron-like spectrum with critical energies between 10 to 20 keV (see Figure 2c) and a total photon yield of 10^9 Photons/eV. To our knowledge, this is the first time that a SMLWFA is shown to generate an x-ray beam of sufficient yield and energy to satisfy the requirements for x-ray absorption spectroscopy measurements of matter driven to extreme conditions.

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Statistical Nonlinear Optics of High Energy Density Plasmas: The Physics of Multiple Crossing Laser Beams

Polymath Research, Inc. ❖ PI: Bedros Afeyan (bafeyan@gmail.com)

The research being carried out by Polymath Research, as part of the Stewardship Science Academic Programs (through the High Energy Density Laboratory Plasmas [HEDLP] Program), is of vital importance in inertial confinement fusion (ICF) research, inertial fusion energy (IFE), high energy density physics (HEDP), and laser-matter interaction (LMI) in general. Due to the coherence of laser radiation, overlapping laser beamlets invariably produce laser hot spots or speckle patterns, or high and low intensity regions with prescribed statistical properties. These act as hotbeds or nucleation sites triggering the spread of instabilities that push plasmas towards large-scale space-time self-organization. This work remedies such catastrophic brushfires and uncontrolled cumulative behavior by taming the behavior of plasmas microscopically while subjected to intense laser irradiation. This method is called Spike Trains of Uneven Duration and Delay (STUD) pulses, where they modulate the laser patterns in space and time in prescribed, deterministic and some random elements (see Figure 1). These act in concert to defeat the plasma's tendency in the presence of excessive and predicable continuous irradiation, to amplify, reflect, and squander the incident energy. That all leads to unpredictable and undesirable behavior such as hot electron preheat or nonuniform, violent, intermittent, bursty behavior. That causes disrupted implosions, as well as ineffective and nonuniform x-ray conversion.

Polymath Research works in close collaboration with Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory, and Sandia National Laboratories scientists on laser-plasma instabilities (LPI) and will be engaging a postdoctoral student in this work this coming year. At the end of two years, the postdoc should be able to join one of the three NNSA national laboratories as the local expert in the STUD pulse program and its implementation.

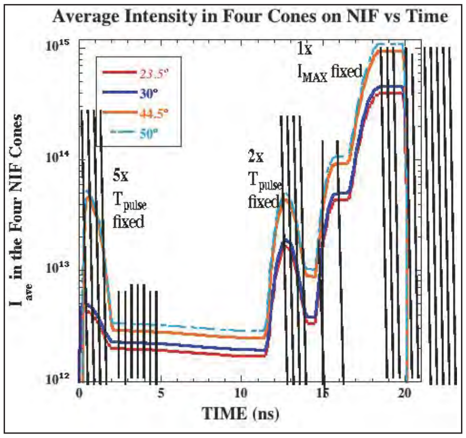

Figure 1. Average intensity in four cones on NIF vs. time for a continuous pulse or a spike train of uneven duration and delay (STUD) pulse superposed. Note that the spikes at different sections of the continuous pulse are different. They either have the same peak intensity as the background and longer duration (I_Max fixed), such as at the last section of the pulse, or the same duration but higher peak intensities (T_Pulse fixed). Each of these three different configurations ensures a proper balance between LPI control capability and laser damage avoidance.

> *"Due to the coherence of laser radiation, overlapping laser beamlets invariably produce laser hot spots or speckle patterns, or high and low intensity regions with prescribed statistical properties. These act as hotbeds or nucleation sites triggering the spread of instabilities that push plasmas towards large-scale space-time self-organization. This work remedies such catastrophic brushfires and uncontrolled cumulative behavior by taming the behavior of plasmas microscopically while subjected to intense laser irradiation."*

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During the first year of this three-year grant, the vital importance of converting the National Ignition Facility (NIF) to GREEN (i.e., the second harmonic) in the near future (as opposed to continuing in the BLUE or third harmonic which is its current configuration) was established. The glass damage threshold is higher, laser bandwidth is significantly increased, and energy available to drive implosions is significantly enhanced. A STUD pulse design made of three distinct pulses was devised. This covered the needs of the front end, middle, and the main drive pulse for NIF targets (see Figure 1). The theory for random phase plate beams which are currently in use on NIF was put forth showing how strongly their catastrophic reflectivity levels can be reduced by using STUD pulses. The new theory covers many different distinct configurations of instabilities that occur in different material complexes in ICF or IFE targets. These theoretical predictions were augmented by numerical simulations that explored complications the theory could not treat easily. These predictions ought to be tested against experiments on the LLNL Janus laser in the coming two years using novel STUD pulse generation designs which were conceived in partnership with scientists at LLNL and which are currently being jointly patented.

Last summer, elements of the STUD pulse program were taught at the HEDP summer school at the University of California, San Diego, by Principal Investigator Dr. Bedros Afeyan. A large number of graduate students learned about the potential of STUD pulses and their benefits for ICF together with sessions on codes and models that can treat complex plasma configurations. Next year's summer school will feature more extensive coverage and highlights of more advanced models bringing the next generation of HEDP scientists in contact with the amount of new laser science together with innovative plasma science needed to crack the ICF and IFE problems for the benefit of humanity at large, and for U.S. national and energy security, in particular.

Development of Talbot-Lau X-ray Deflectometry Density Diagnostic

Johns Hopkins University ❖ PI: Dan Stutman (dstutman@jhu.edu), Author: Maria Pia Valdivia (mpvaldivia@pha.jhu.edu)

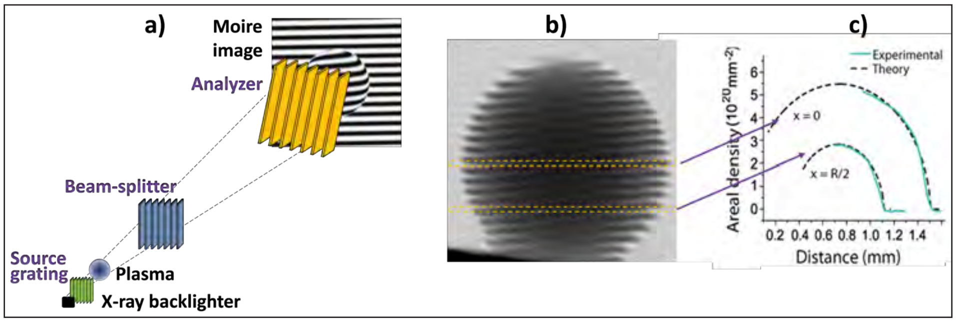

Figure 1. a) Layout of Talbot-Lau deflectometer, b) Image of Moiré fringe shift produced by a PMMA sphere at 8 keV, c) Experimental and theoretical areal electron density in two cross sections.

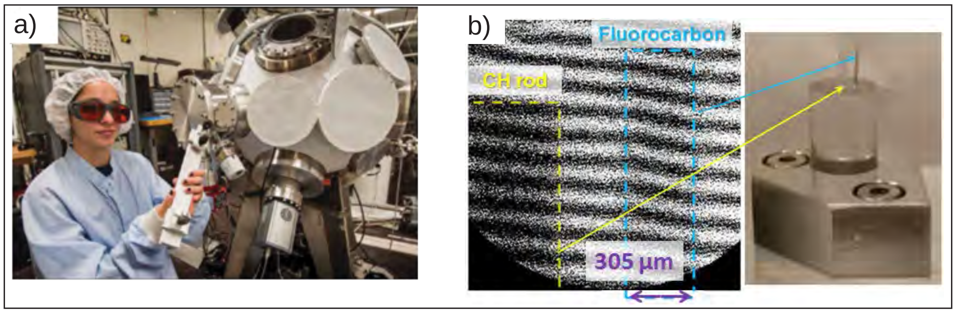

Figure 2. a) Installation of the TXD interferometer at MTW, b) Moiré images of plastic rods obtained with a Cu K-α foil backlighter.

The Johns Hopkins Plasma Diagnostic Group has developed Talbot-Lau x-ray deflectometry (TXD), a novel electron density diagnostic for high energy density plasmas (HEDP). Graduate and undergraduate students have been supported, through collaborations, under SSAP sponsorship (through the High Energy Density Laboratory Plasmas program). Principal Investigator Dan Stutman notes: “Students involved in our program have the opportunity to develop an entirely new measurement technique. They can study and test this new diagnostic in the laboratory as well as in the HEDP environment.”

TXD measures micro-radian angular deviations caused by x-ray refraction.[1] These x-rays can be generated by laser- or pulsed discharge-driven backlighters, with energy 8-17 keV.[2,3] The spatial resolution in TXD is limited by the x-ray backlighter source size, to >10 μm. The refraction angles provide maps of the plasma electron density gradient, and after integration, electron density maps. X-ray absorption, refraction, and small-angle scatter are measured simultaneously. The average line-of-sight plasma composition can also be deduced.[4]

The layout of a high magnification Talbot-Lau interferometer is shown in Figure 1a. The source grating transforms an incoherent x-ray source into an array of spatially coherent sources that illuminate a phase grating. The phase grating produces a microscopic fringe pattern, through the Talbot effect, at the analyzer grating. A macroscopic Moiré fringe pattern is obtained by rotating one of the gratings. The x-ray refraction angles are retrieved from the Moiré pattern by comparing with a reference image in the absence of plasma. Figures 1b and 1c show Moiré images of a 1.5 mm PMMA sphere at 8 keV, and its measured and theoretical electron density profiles.

The technique has recently been demonstrated at the University of Rochester Laboratory for Laser Energetics (see Figure 2a). Foil, micro-wire, and micro-sphere x-ray backlighter targets were successfully tested for TXD.[2] Moiré images of thin plastic rods obtained are shown in Figure 2b. Source grating survival was demonstrated for grating-to-target foil distances of ~1-3 mm. Experiments in collaboration with Pontifica Universidad de Chile demonstrated that TXD can be implemented using x-pinches as x-ray backlighters suggesting that TXD can be utilized in pulsed power environments.[2]

A first plasma experiment at OMEGA-EP is planned for 2018, to measure the electron density profile of a planar CH plasma produced. Once benchmarked, electron density mapping through TXD, together with its additional features, will help us understand ablation dynamics in laser-produced coronal plasmas, and validate simulation codes.

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Jessica L. Shaw, Laboratory for Laser Energetics, University of Rochester (jshaw05@lle.rochester.edu)

Years at LLE: 2016-Present ❖ Degree: PhD, Electrical Engineering ❖ SSAP Program: 2010-2016, University of California, Los Angeles

Since first walking across a sticky mat and into a laser lab during a summer internship, I knew I wanted to build my career as a researcher in the field of laser-plasma interactions (LPI) and plasma physics. Studying those fields was intellectually challenging, and it was both humbling and exciting to work with some of the brightest minds in the field. Experimenting at an NNSA laboratory meant that the research not only advanced fundamental science but also contributed to the knowledge and scientific techniques needed to fulfill the laboratory's mission. After this internship, I was certain that I wanted to build a career at a laboratory affiliated with NNSA, but I still had much to learn.

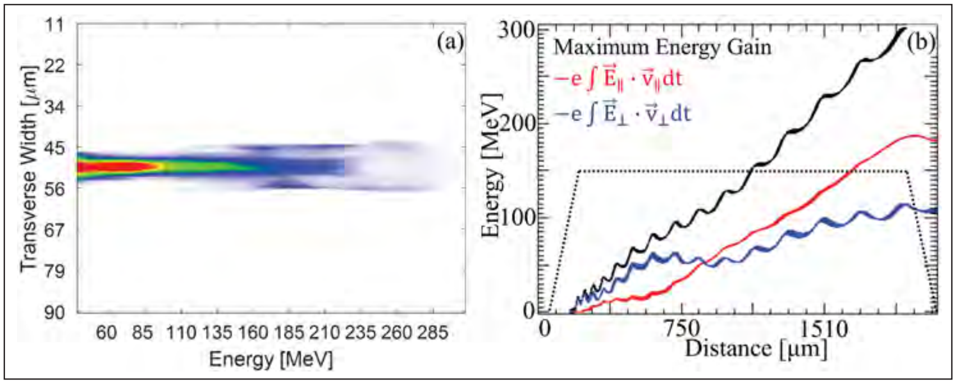

Figure 1. (a) Simulated electron spectrum from a two-dimensional particle-in-cell simulation of a LWFA where the laser pulse overlaps the trapped electrons. The electrons are dispersed orthogonal to the laser polarization, and the resulting forked structure seen at the higher energies of the electron spectrum is characteristic of the presence of DLA in LWFA.[1] *(b) Plot of the maximum energy gain (black curve), LWFA contribution (red curve), and DLA contribution (blue curve) for the highest-energy electrons in (a).*[2] *The curves show that those electrons gain significant energy from dual acceleration mechanisms—DLA and LWFA. The electron spectrum and calculations are from a simulation completed with OSIRIS of a 45 fs laser pulse with an a_0 of 2.1 propagating through 1,800 μm of 8 x 10^{18} cm^{-3} plasma. The dotted black curve in (b) marks the plasma density profile.*

To prepare for a research career, I sought a PhD program that included hands-on LPI and plasma physics research and close mentorship, but also provided broad access to the wider physics community. Professor Chan Joshi's Plasma Accelerator Group at the University of California, Los Angeles (UCLA) met all those qualifications. The backbone of my graduate work at UCLA was the daily interactions with an experienced plasma physics research team and weekly research meetings where students would present their research progress. Giving weekly research presentations in front of a knowledgeable and critical, but supportive, audience transformed me into a confident presenter and sharpened my ability to think on my feet. At these research meetings, I received an in-depth and sustained exposure to a variety of fields from plasmas to accelerators to nonlinear optics to laser science. My dissertation research was completed at one of Professor Joshi's laser laboratories at UCLA, and during this hands-on work, I was closely mentored by staff scientists. My graduate education was enriched by many opportunities to travel to NNSA laboratories to collaborate with scientists from both national laboratories and world-class universities. My dissertation research [1] on the presence of direct laser acceleration (DLA) in laser wakefield accelerators (LWFA) (see Figure 1) played a key role in interpreting data from a recent collaborative UCLA/Lawrence Livermore National Laboratory (LLNL) experiment. I was also given the opportunity to travel to many conferences, workshops, and summer schools. These scientific gatherings offered the opportunity to present my dissertation and collaborative work and to closely follow the status and trends of the research field, including the work being conducted at the various laboratories.

The broad background that I developed and the exposure at NNSA national laboratories and NNSA-funded laboratories that I received as a graduate student in Professor Joshi's group has been vital in my new role as a Scientist at the University of Rochester Laboratory for Laser Energetics (LLE). My background enables me to understand the diverse research conducted at the NNSA-supported LLE and to assess how my expertise can benefit that current research and contribute to LLE's mission. One of my main projects at LLE is to develop compact, directional x-ray sources. Currently, I am working to demonstrate betatron x-ray sources driven by picosecond-scale, kilojoule-class lasers that are found in conjunction with the large-scale facilities conducting inertial confinement fusion (ICF) research such as the National Ignition Facility at LLNL, OMEGA at LLE, and the Z machine at Sandia National Laboratories. This research will extend the work begun through the UCLA/LLNL collaboration on LWFA-produced x-ray sources while simultaneously bringing a new experimental platform and diagnostic capability to LLE. X-ray radiography plays a key role in obtaining data on the performance of ICF experiments, and x-ray probing diagnostics are important to many other fields of science, from astrophysics to material science to biology. Betatron x-ray sources may be useful for the realization of 20-80 keV-class directional x-ray beams in the near future.

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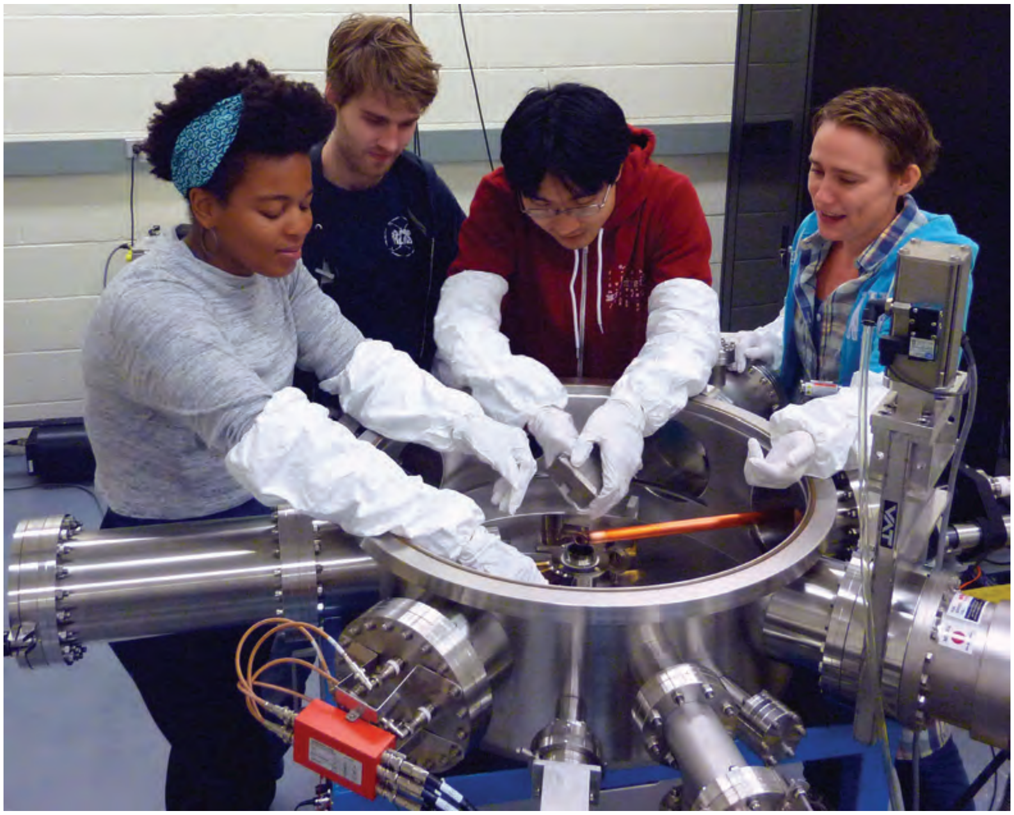
“The [Johns Hopkins Plasma Diagnostic] Group has developed Talbot-Lau x-ray deflectometry (TXD), a novel electron density diagnostic for high energy density plasmas (HEDP). Graduate and undergraduate students have been supported, through collaborations, under SSAP sponsorship (through the High Energy Density Laboratory Plasmas program). Principal Investigator Dan Stutman notes: “Students involved in our program have the opportunity to develop an entirely new measurement technique. They can study and test this new diagnostic in the laboratory as well as in the HEDP environment.”

* * *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Non-Linear Amplification of Magnetic Fields in Laser-Produced Plasmas

University of Chicago ❖ PI: D.Q. Lamb (lamb@oddjob.uchicago.edu)

Figure 1. Top: Group photo from one of our shot days at the Omega Laser Facility with two of our graduate students, Jena Meinecke (second from right, front row), and Alexandra Rigby (third from right, front row). The program also provided crucial support for graduate student Archie Bott and postdoctoral scholars Laura Chen and Thomas White. Bottom left: The group working in the strategy room at the OMEGA laser. Bottom right: The "forest" of targets we fielded on our shot day.

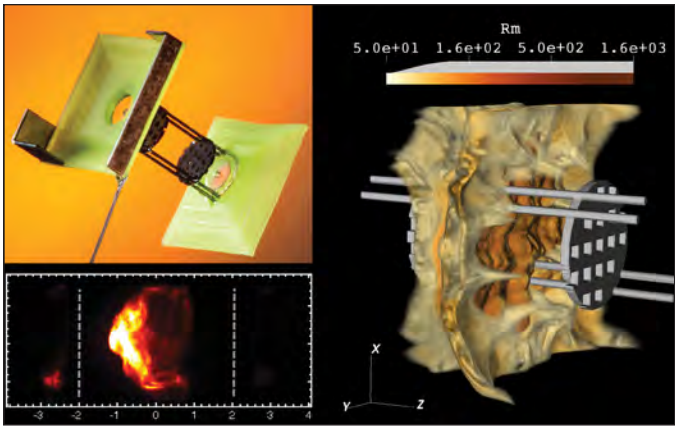

Figure 2. Top left: A close-up of the experimental target. Bottom left: X-ray image of the interaction region after collision. Right: FLASH simulation of the experimental platform, showing the simulated magnetic Reynolds number after collision.

Magnetic fields thread our universe up to the largest observable structures, which are galaxies and galaxy clusters. While a number of theories have been put forward to explain how cosmic "seed" magnetic fields are generated, the way these fields are amplified to the values we observe today is thought to be the turbulent dynamo mechanism. This mechanism has eluded experimental demonstration for decades, as it requires large magnetic Reynolds numbers (Rm) to operate. The Turbulent Dynamo (TDyno) National Laser Users' Facility (NLUF) project is an international collaboration led by the University of Chicago and the University of Oxford that aims to demonstrate and study turbulent dynamo in a controlled laboratory environment. It capitalizes on a five-year experimental effort that studied magnetized turbulence in small-scale laser facilities,[1,2] and leverages FLASH, a publicly available three-dimensional (3D) radiation-magnetohydrodynamic simulation code we have developed, which can accurately model laser experiments of laboratory plasmas.[3] Under the auspices of SSAP, through the NLUF program, we designed and conducted experiments with the OMEGA laser at the University of Rochester Laboratory for Laser Energetics that reached the required large Rm-regime. The NLUF program provided critical support for training young scientists (see Figure 1)—graduate students Jena Meinecke, Alexandra Rigby, and Archie Bott, and postdoctoral scholars Laura Chen and Thomas White. This support also enabled their participation in our two OMEGA shot days and their attendance in large international conferences, where they presented the results of our experiments. University of Chicago undergraduates Jordan Laune and Christopher Walker are working on simulation projects related to these experiments.

"The NLUF program has made possible exciting new science and has provided crucial support for training the new generation of HEDP scientists," said Principal Investigator D.Q. Lamb.

The TDyno NLUF project brings together experts in experiments, theory, and numerics. Aided by 3D FLASH simulations on Argonne National Laboratory's *Mira* BG/Q supercomputer, we designed an OMEGA experimental platform (see Figure 2) that is uniquely suited to generate turbulent plasmas in the large-Rm regime, where dynamo can operate. The platform consists of two diametrically opposed foil targets that are backlit with temporally-stacked OMEGA beams, which deliver 5 kJ of energy on each side. The beams drive a pair of plasma flows that carry seed magnetic fields generated by the Biermann battery effect, an effect where the weak seed field is generated by relative motion between electrons and ions. The flows propagate through a pair of grids and meet at the center of the OMEGA chamber to form a hot, turbulent interaction region where seed magnetic fields are amplified to magnetic energies that are on par with the turbulent kinetic energy, as occurs in cosmic magnetic fields.

We collected a wealth of experimental data that characterizes the magnetized, turbulent plasma, and reveals the distribution of turbulent energy among velocity, magnetic field, and density fluctuations. Amplification of the seed magnetic fields was measured using proton radiography and Faraday rotation. The TDyno NLUF project has furthered our understanding of turbulent dynamos and has trained young scientists in the design, execution, and interpretation of laser-driven high energy density physics experiments—a critical national need.

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Hot Electron Scaling in Long Pulse Laser Plasma Interaction Relevant to Shock Ignition

General Atomics ❖ PI: M.S. Wei (weims@gat.com)

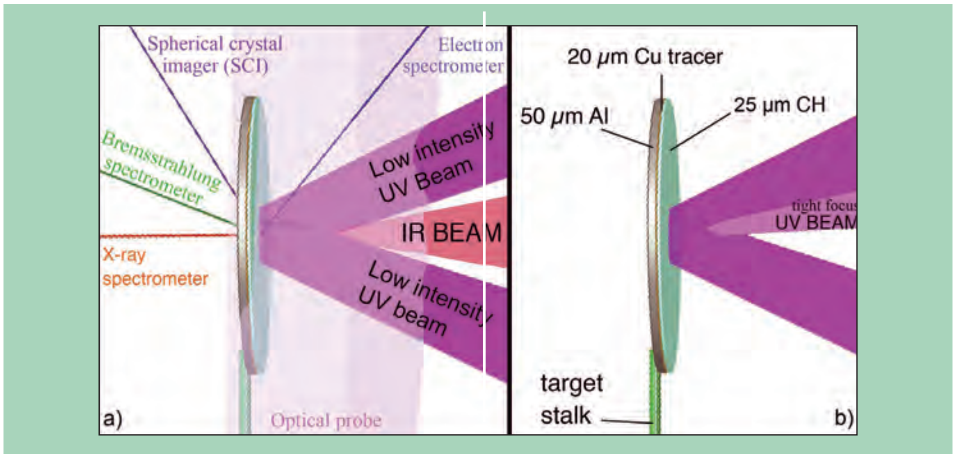

Figure 1. Experimental design with (a) 100-ps IR beam (up to 2.5 kJ energy) and (b) 1-ns UV beam (~1.3 kJ energy) as the high intensity interaction beam, respectively.

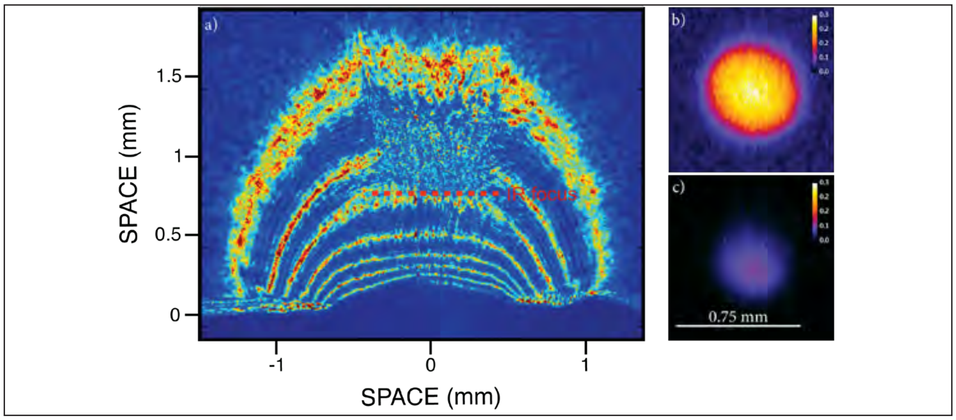

Figure 2. (a) Optical probe AFR data showing the propagation of the IR beam in long scalelength underdense plasma; 2D images of hot electron-produced Cu Kα radiation from (b) the high intensity IR interaction and (c) the low intensity UV beams, respectively.

Shock ignition (SI), an alternative high-gain laser fusion scheme, requires launching a strong shockwave into already moderately compressed fuel to achieve ignition. This late-time shock generation requires a short-duration (0.5-1 ns) high intensity laser (>5×10^{15} W/cm^2) interacting with a long scalelength plasma and subsequent coupling energy to the high density SI target. Copious hot electrons produced from laser plasma instabilities (LPI) in this regime may be detrimental or advantageous to the system depending on their energy. This NNSA-funded, General Atomics-led National Laser Users' Facility project investigates the hot electron scaling as a function of laser wavelength, intensity, and plasma conditions that are pertinent to SI target physics. Collaborating with researchers from the University of California, San Diego and the University of Rochester, the project supports the training of two graduate students and two postdoctoral fellows from these institutions.

Figure 1 shows OMEGA EP experimental design with planar targets that use two large-spot low intensity (4 ns, 3.5×10^{14} W/cm^2) ultraviolet (UV:0.351 μm) laser beams irradiating a multilayer (CH/Cu/Al) foil to create the large-scale hot plasma of interest. This is followed by the injection of a high intensity interaction beam, either a 100-ps infrared (IR: 1.053 μm) beam or a 1-ns UV beam, ranging from 1.6×10^{16} to 2.6×10^{17} W/cm^2 at various time delays as proxy for the ignitor pulse in the SI scheme. This high intensity beam was focused with ~100 μm spot size at its corresponding quarter critical density (n_c/4) region. The plasma LPI phenomena were characterized by the angular filter refractometry (AFR) using the 10 ps optical probe. Fast electrons' energy and spatial distributions were characterized via measuring the induced Cu K-shell fluorescence and bremsstrahlung radiation.

At the highest vacuum intensity of 2.6×10^{17} W/cm^2, the normal incident IR beam with 2.5 kJ energy can be seen strongly interacting with the underdense plasma in the range of n_c/10 to n_c/4 in the AFR data and then breaking into many filaments (see Figure 2a). These laser filaments appear to propagate all the way to the critical density (n_c) without merging. In contrast, the high intensity UV beam having an incident angle of 23° was found to be refracted out of the central target plasma as it propagated through density gradients in both axial and radial directions. The measured Cu Kα radiation by a spherical quartz crystal imager and a x-ray spectrometer showed a significant increase (~400%) due to the IR beam-produced hot electrons (see Figure 2b) compared to the background shot with just the lower intensity plasma creation beams (see Figure 2c). The high intensity UV beam interaction only produced a small increase (35%), confirming poor coupling. In the IR case, laser filaments may be producing and/or guiding hot electrons evidenced by the 465 μm Kα spot, which is comparable to the overall size of the filamentary beam seen in Figure 2a. Analysis of the hard x-ray spectrum data suggests the IR beam-produced hot electrons have a temperature T_{hot} ~70 keV for an exponential energy distribution with the laser-to-electron energy conversion efficiency of a few percent. This first time data is encouraging for electron assistance in the SI concept. LPI, including filamentation and hot electron generation, have also been observed in the ongoing two-dimensional (2D) particle-in-cell modeling of the experiments. Detailed analysis and journal publications are underway.

Electron Acceleration from Underdense Plasmas

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Co-investigators: A. Hussein, A. Raymond, K. Krushelnick (University of Michigan), P. Nilson, D. Froula, D. Harberberger, A. Davies, W. Theobald (University of Rochester Laboratory for Laser Energetics), J. Williams, H. Chen (Lawrence Livermore National Laboratory), A. Arefiev (University of Texas)

The generation of energetic electron beams from intense laser plasma interactions has potential applications ranging from high resolution x-ray radiography of fusion targets to high energy physics experiments. In FY 2016, studies of direct laser acceleration mechanisms and laser channeling in underdense plasmas were conducted using the OMEGA EP laser.

An underdense plasma was formed by ablation of a 1000 µm plastic foil having a 400 µm hole drilled through the center with a 1000 J nanosecond pulse length UV laser. Plasma was allowed to propagate toward the center of the target, where a picosecond 400 J, 1.053 um pulse was focused onto the plasma plume. This target was designed to prevent electron beam pointing instabilities due to density gradients. A laser channel was formed in the target due to the expulsion of plasma from the laser axis from ponderomotive force effects. This channel was then imaged using proton beam probing produced via the interaction of a 250 J, 10 ps infrared pulse with a Cu foil. Images were taken of the laser channel at different times in the plasma formation, both with and without the short pulse infrared beam interacting with the plasma. The scale length of the channel in this target geometry was found to be roughly 5 times shorter than the lengths of channels observed in other configurations.[1] In addition to measuring the geometry of the plasma channel, the proton probe was able to temporally resolve the evolution of the channel and the appearance of hot electrons to within 5 ps. This time scale allowed the observation of the emergence of "sheath" field driven by hot electrons which propagated out from the main interaction point at approximately 0.1 c. This feature was not observed when the short pulse infrared beam was not fired (see Figures 1a and 1b). A feature indicative of a jet of hot electrons (circled in red in Figure 1b) was also seen exiting the target slightly above the direction of laser propagation.

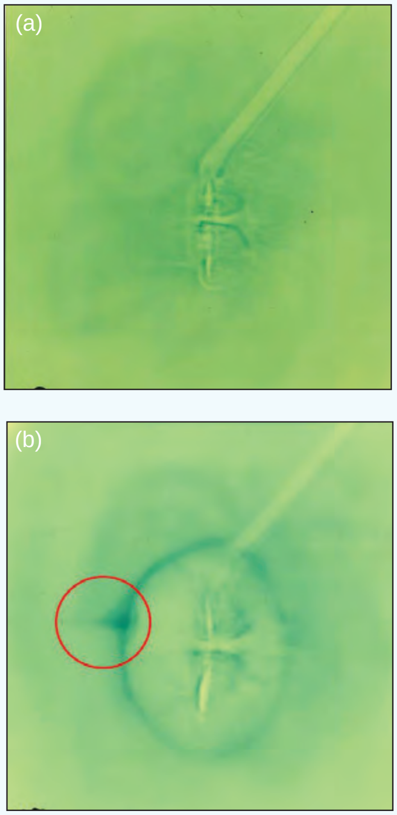

Figure 1. (a) Proton probe image of preformed expanding plasma. (b) Proton probe image of high intensity interaction, with preformed plasma. The ring feature is a region of high electric field associated with the hot electrons from the main interaction beam. The OMEGA EP laser is incident from the right.

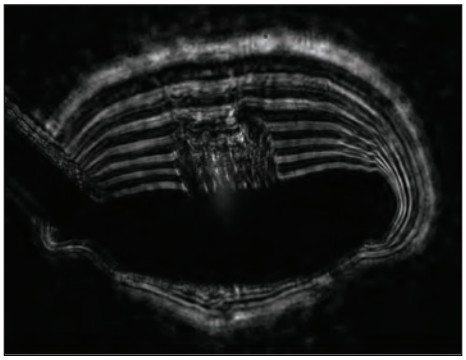

Figure 2. Angular filter refractometry of preformed plasma plume expansion.

> *"The generation of energetic electron beams from intense laser plasma interactions has potential applications ranging from high resolution x-ray radiography of fusion targets to high energy physics experiments. In FY 2016, studies of direct laser acceleration mechanisms and laser channeling in underdense plasmas were conducted using the OMEGA EP laser."*

* * *

In addition, the 4ω optical probe diagnostic was used to view the plasma expansion. The angular filter refractometry diagnostic measured the degree of refraction of the 263 nm probe beam passing through the plasma during the interaction. From this information, the plasma density profile was obtained.

The electrons which propagated to the spectrometer were accelerated via Direct Laser Acceleration in the channel and were measured to have a broad spectrum with a peak energy of about 50 MeV. The features of channel formation were observed with the proton probe and optical diagnostics.

Future work will focus on optimizing the plasma density for electron acceleration to much higher energies as well as measurements of x-ray production and source size. In addition we will studying the effect of plasma density on the channel formation dynamics and dimensions.

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Years at LLE: 2015-Present ❖ Degree: PhD, Physics ❖ SSAP Program: 2008-2014, Massachusetts Institute of Technology

The National Laser Users' Facility (NLUF) program was vital to my graduate studies in the High Energy Density Physics (HEDP) division at the Massachusetts Institute of Technology (MIT), under the supervision of Dr. Richard Petrasso. My thesis was based on several experiments at the OMEGA and OMEGA EP lasers at the University of Rochester Laboratory for Laser Energetics (LLE). The NLUF program allowed me and my collaborators to make significant advances in HED science, relevant to both inertial confinement fusion (ICF) and fundamental science, and brought me in contact with outstanding scientists at LLE and other NNSA national laboratories and universities, leading to my employment at LLE today. Based on my work, I was fortunate to be selected for the 2016 Marshall N. Rosenbluth Outstanding Doctoral Thesis Award, a reflection of the caliber of research enabled by the NLUF program.

My research included a demonstration of ion kinetic effects during the shock-convergence phase of ICF implosions. By varying plasma conditions across different experiments, regimes where hydrodynamics is valid, and alternatively where ion kinetic effects are expected to be important, were investigated. Measured fusion yields increasingly deviated from the predictions of hydrodynamics simulations as the ion-ion mean free path became longer, a signature of ion kinetic effects.[1]

I additionally investigated the reconnection of magnetic fields at high densities and strong flows, a little-explored regime relevant to space- and astro-physics phenomena. Laser-foil interactions generated oppositely-directed magnetic fields, which were then driven to collide, causing magnetic field annihilation or reconnection. On OMEGA, the inferred magnetic flux annihilation rate was found to be fast and dictated by the flow velocity.[2] These first experiments investigating magnetic reconnection with an asymmetric collision found similar results to experiments driven symmetrically.[2] On OMEGA EP, protons generated by the interaction of a short-pulse laser with a foil target were used to radiograph a magnetic reconnection (see Figure 1). The images shown illustrate both the formation of plasma jets ejected into the outflow region (see Figure 1c), and the persistence of a stable current sheet (see Figures 1d and 1e) at late times, signifying an evolution in magnetic reconnection regime from fast (collisionless, strongly driven) to slow (collisional, weakly driven).[3]

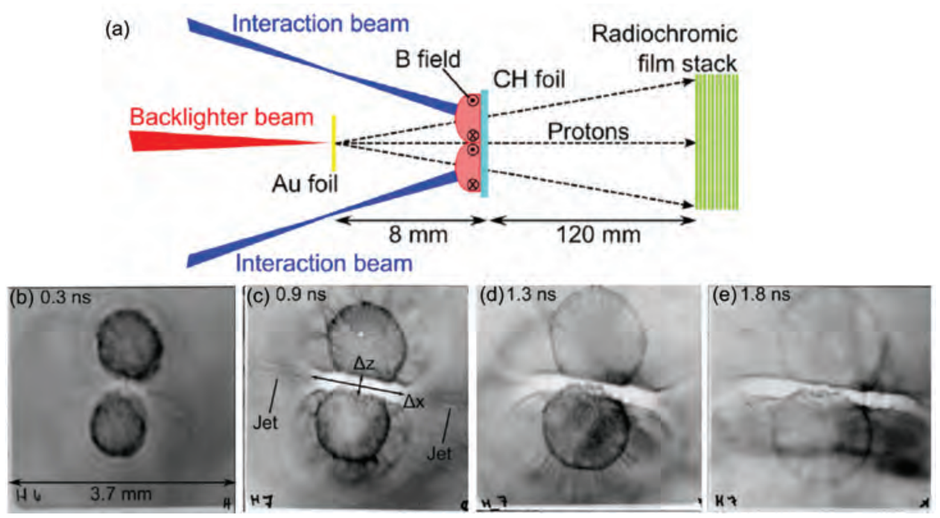

Figure 1. (a) Experimental setup for proton radiography of magnetic reconnection on the OMEGA EP laser system. Proton radiography images generated by (b) 18-MeV or (c-e) 24-MeV protons illustrate the formation of plasma jets at early times and the persistence of a stable current sheet (light region) at late times.

Based on my excellent experience and my many fruitful and enjoyable collaborations throughout my graduate work, I am continuing my career towards the compelling problem of achieving fusion ignition in the laboratory. I am currently a research associate at LLE, implementing experiments on the National Ignition Facility (NIF). Leading the LLE-led direct-drive campaign on the NIF, I work with experts from several institutions to understand laser-plasma interactions at direct-drive ignition-relevant scales, as they affect laser energy coupling and target preheat. We intend to evaluate the viability of direct drive as a potential avenue for achieving ignition on the NIF.

The NLUF program, with the opportunities it affords to conduct experiments at world-class facilities and to interact with top scientists in the field, is a unique resource of lasting value to both students and the national ICF program alike.

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Suzanne Ali, Lawrence Livermore National Laboratory (ali3@llnl.gov)

Years at LLNL: 2011-Present ❖ Degree: PhD, Physical Chemistry ❖ SSAP Program: 2009-2015, University of California, Berkeley

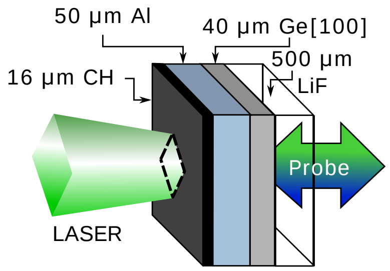
I received my graduate degree at the University of California, Berkeley with Professor Raymond Jeanloz. The dynamic compression experiments were fascinating for their challenges: the scale over which they occur, their difficulty, and the limited opportunities for repeatability.

I primarily worked at the Jupiter Laser Facility at Lawrence Livermore National Laboratory (LLNL). I'm very grateful for the guidance of the researchers and the support from the Stewardship Science Academic Programs (through the National Laser Users' Facility program). This flexible facility allowed complex diagnostic and technique development, despite the time constraints of campaign experiments. I gathered enough experience to develop my own diagnostic, the Shock Wave Optical Reflectivity Diagnostic (SWORD) which allows us to measure broadband reflectivity across the visible and near-infrared with 10 nm spectral and 0.5 ns temporal resolution, and is crucial for characterizing changes in chemical bonding and the associated electronic structure.[1] The figure illustrates the target design and results from the SWORD.

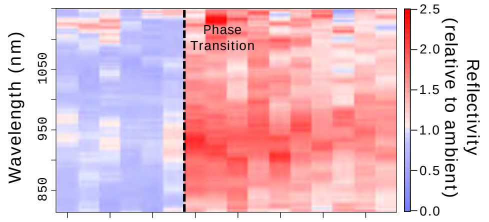
The NLUF program allowed me to work on a broad range of experiments, with both academic and NNSA national laboratory collaborators. I used a velocimetry diagnostic[2] to study diamonds, helped develop a technique to measure transverse velocities in shock-compressed samples, and fielded the SWORD to help characterize phase transitions in alkali metals.

As a postdoctoral researcher at LLNL, I am working on an analysis technique to decouple the many parameters that contribute to the measured material response in dynamic compression experiments, and investigating the hydrodynamic response of capsule ablator materials. In addition to the technical opportunities provided by working at a national laboratory, the people at LLNL have been a huge part of why I chose to continue at the laboratory. As a graduate student, it is incredibly useful to be connected to a network of people with a variety of specialties and fields of interest, all of whom have been extremely helpful.

(a) Target Schematic



(b) Reflectivity Spectra



(c) Reflectivity at 925 +- 25 nm

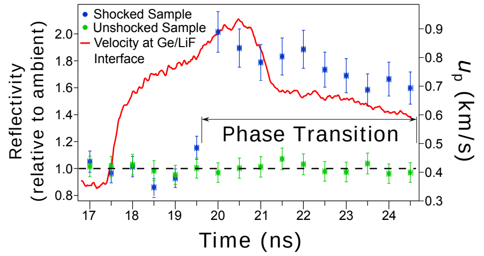


Figure 1. (a) Target design for the discussed experiments. The material of interest, germanium, was sandwiched between a lithium fluoride window and an aluminum pusher with an ablative plastic layer on the drive side. (b) Reflectivity spectra from the SWORD. Following elastic wave arrival at 15 ns and inelastic wave arrival at 17.5 ns, there was a small decrease (5%-10%) in the intensity of the sample pulses, probably due to a roughening of the target surface. An 80%-90% increase in the reflectivity of the sample occurred at 19.5 ns, indicating the germanium phase transition accompanied by closure of the band gap. (c) Reflectivity between 900 and 950 nm extracted from (b). The small decrease in reflectivity that accompanied the elastic and inelastic precursors can be observed between 17 and 19 ns, with the significant increase that accompanied the phase transition beginning at 19.5 ns. The dashed black line at a reflectivity of one is a guide for the eye. The red line is particle velocity at the germanium-LiF interface obtained from velocimetry. The elastic wave begins prior to the SWORD time window, but the rise of the inelastic wave can be seen at 17.5 ns and the arrival of a phase transition wave can be observed at 19.5 ns.

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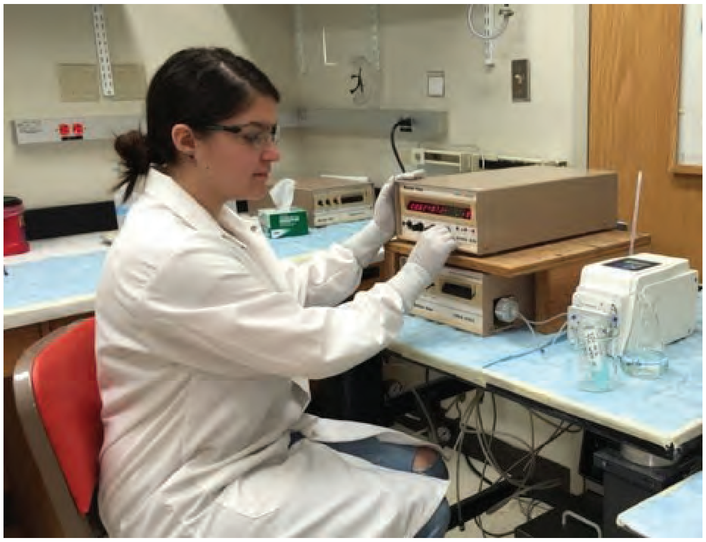

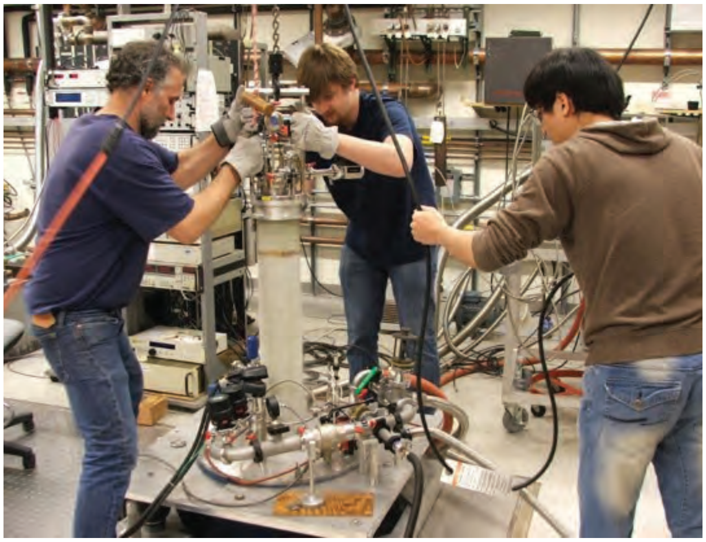

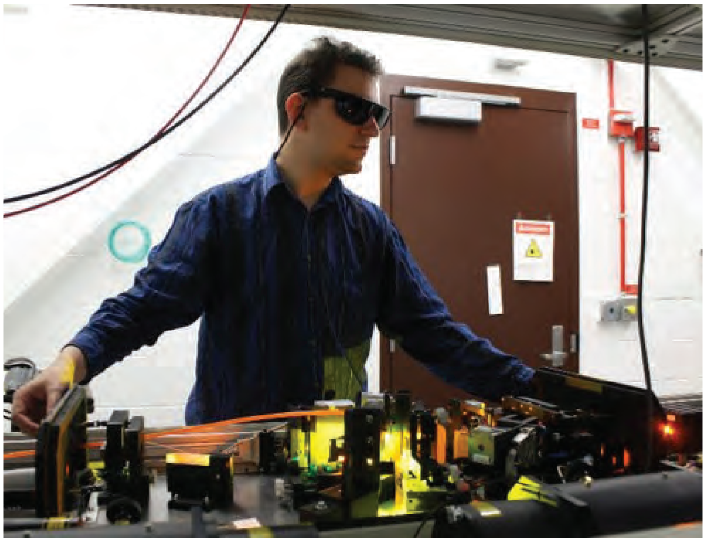

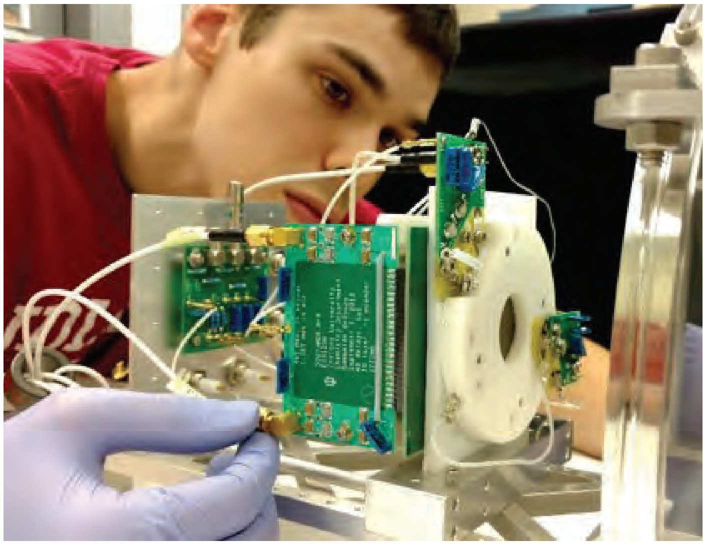

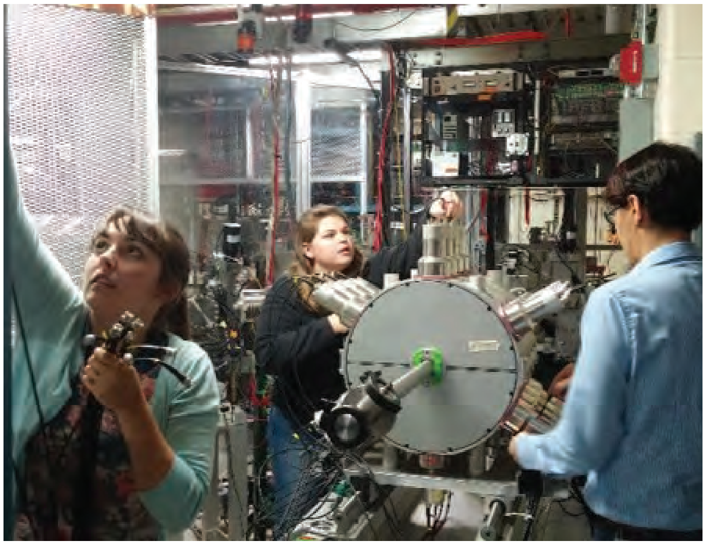

Jerrad Auxier, University of Tennessee, Knoxville (jauxier1@vols.utk.edu, jpauxier@lanl.gov)

Degree in Progress: PhD, Nuclear Engineering ❖ University Advisor: Dr. Howard L. Hall ❖ SSAP Program: 2013-Present

Research Topic

Nuclear forensics and security

What are your research responsibilities?

During the past few years conducting research under the SSAP, I have been responsible for developing computer models to produce high fidelity post-detonation surrogate debris. In order to produce accurate surrogate melt glass, it was vitally important to create a high fidelity computer model that would account for all possible blast effects in the event of a nuclear detonation to accurately predict the composition of fallout.

How have you benefitted from the SSAP?

By being a participant of an SSAP research team, I have developed skills and knowledge that equip me for future employment, such as my position at Los National Laboratory (LANL). During my first year at LANL, I utilized research expertise which I had developed in the SSAP program. After completing my second year of graduate school under the SSAP, I was hired at LANL as a post-master candidate to help model criticality curves for varying composition plutonium spheres. While at LANL, the R&D engineers were instrumental in the development of my PhD project. With the opportunities that SSAP has provided me, I can look forward to a bright future in the field of Nuclear Forensics in hopes of bettering the world we live in.

Have you spent time at one of the national laboratories?

Because of the research I have completed at the University of Tennessee in conjunction with the SSAP program, I was hired for two consecutive summers at LANL. I have had the opportunity to collaborate with staff scientists and engineers who have assisted me in developing my PhD project in Nuclear Forensics. Having the opportunity to work at a NNSA national laboratory has given me, as a student, the ability to brainstorm ideas and discoveries with the leading researchers in my field of expertise. They have made suggestions and given me advice on ways to improve my project to make it more relevant in the area of Nuclear Forensics. Since LANL is one of the most respected national laboratories, my experience there gives me greater employment opportunity. As I submit resumes and complete job interviews, I find that my association with LANL gives me more credibility as a possible employee.

Tom Byvank, Cornell University (tb395@cornell.edu)

Degree: PhD, Applied and Engineering Physics ❖ University Advisor: Professor Bruce Kusse ❖ SSAP Program : 2013-Present

Research Topic

Magnetized plasma jets experiments and simulations

What are your research responsibilities?

I research the effects of magnetic fields on laboratory plasma jets, and I compare experimental results with simulation predictions. A pulsed power machine creates the plasma jets from solid foils, and I study the dynamics of the plasma density, temperature, velocity, and magnetic field compression utilizing diagnostics, including interferometry, Thomson scattering, and magnetic Bdot probes. I also study how the ablation of different foil materials impacts the plasma jet behavior. Additionally, by changing the direction of current flow through the plasma jet, I compare the experimental jet structure with extended magnetohydrodynamic (XMHD) numerical simulations that I run. The simulations validate that the Hall term in the Generalized Ohm's Law influences the plasma dynamics as is observed in the experiments.

How have you benefitted from the SSAP?

The SSAP supports the facilities to provide me with a hands-on learning experience to set up experiments, make mistakes, and learn from my mistakes. The funding has allowed me to present posters and talks across the country as well as internationally. Furthermore, the SSAP connects me with a network of scientists who can share their expertise, constructively criticize my work, give me feedback for improvement, and teach me about their own research.

Have you spent time at one of the national laboratories?

I spent the summer of 2016 as a graduate intern at Sandia National Laboratories (SNL) in the High Energy Density Experiments group. The internship allowed me to get a feel for the large collaboration efforts needed to conduct research at world-class facilities like the Z machine. My experience provided further motivation for my interest in comparing experiments with simulations, learning both from when they agree and also from when there are discrepancies. Furthermore, I was able to use an MHD code and the computing resources at SNL to help build my intuition regarding some aspects of my thesis work of observed experimental material-dependent instabilities. Overall, I left my internship inspired and validated that I enjoy the challenges of plasma physics research, and I was impressed by the resources and opportunities facilitated by national laboratories. Last but not least, my time in Albuquerque let me explore the beautiful nature of New Mexico.

Wei-ting Chiu, University of California, Davis (wtchiu@ucdavis.edu)

Degree: PhD, Condensed Matter Physics ❖ University Advisor: Professor Richard Scalettar ❖ SSAP Program: 2015-Present

Research Topic

Calculation of the x-ray emission spectrum from light Lanthanide Metals

What are your research responsibilities?

Some Lanthanide metals undergo a volume collapse transition (VCT) at certain pressure. Two competing theories of the VCT are (1) the Mott-Hubbard model which suggests a vanishing *f* moment above the transition whereas (2) the Kondo model which has a stable *f* moment across the VCT. High pressure x-ray emission spectroscopy is a useful tool to understand the physics of this phenomenon. The spectra are measured by our collaborators from Lawrence Livermore National Laboratory (LLNL) and the University of Washington. They use a diamond anvil cell to apply different pressures on cerium, praseodymium, and neodymium, and then take the x-ray emission spectra for each material. My work, with collaborators from Stanford University, is to calculate the spectra using an extended atomic model. The model includes a single atomic site with partially-filled f shell hybridized with conduction bands. Using high energy x-rays, one can excite an electron to vacuum and create a 2p core-hole at the site. After a non-resonant x-ray emission, the core-hole is recombined with a higher energy *4d* electron and leaves another core-hole. All the multiplet interactions between the core-hole and outer-shell electrons are taken into account in the model. Our results show that the *f* moments for cerium and praseodymium are stable across the VCT. Thus, the Kondo model is suitable for explaining the VCT in these two materials.

How have you benefitted from the SSAP?

The funding from NNSA allowed me to focus on my research and be able to attend the APS March meeting in 2015. Thanks to it, I could give a talk to people about my research and learn a lot of advanced physics from the talks by top researchers and professors. This program provides me a great opportunity of broadening and deepening my knowledge.

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

Yes. As a theorist the chance of doing experiments is rare, but knowing what the experiment is doing is important. This program allows me to work with experimentalists and learn most of the details about the x-ray emission experiments from them. Also, Professor Tom Devereaux's group provides a lot of help in the theory part of my research. This collaboration combining theory and experiments gives me a precious experience of doing research.

Ginevra Cochran, The Ohio State University (cochran.339@osu.edu)

Degree: PhD, Physics ❖ University Advisor: Dr. Douglass Schumacher ❖ SSAP: 2014-Present

Research Topic

Short pulse laser-matter interactions, experiments and simulations

What are your research responsibilities?

I study the interaction of ultrashort laser pulses with plasmas, both experimentally and through simulations, with my current focus being ion acceleration. I participate in laser ion acceleration experiments at The Ohio State University's (OSU's) Scarlet laser, as well as at other facilities, and I am one of the team of graduate students which helps run Scarlet. I also have primary responsibility for designing and running particle-in-cell simulations to analyze our results. These simulations allow insight into the short timescale dynamics that our detectors cannot resolve. I have also developed simulations of pulse-cleaning plasma mirrors which I have benchmarked against experimental results. Most recently, I lead a four-person experimental team of graduate and undergraduate students working to expand the liquid crystal target technology developed at OSU to other ultra-intense laser applications.

How have you benefitted from the SSAP?

In addition to direct support for me, the SSAP has provided me with many opportunities to broaden my scientific skillset. The largest of these is access to the Scarlet laser itself, which was constructed under an NNSA grant and operates under SSAP support. Working with Scarlet has provided me with a valuable chance for hands-on experience with a petawatt-class laser, not only designing and running experiments but with laser operation, diagnosis, and development. SSAP funding has supported a wide range of experiments at Scarlet that I have been able to participate in, ranging from studies of structured targets to ultrathin target work which allows investigation of novel acceleration mechanisms. Support from the SSAP has also allowed me to travel to conferences like the SSAP Symposium and the APS Annual Division of Plasma Physics, where I can both present my research and learn about that of others.

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

One of the most beneficial aspects of my SSAP support has been the ability to collaborate and consult with scientists at other institutions. As one example, we have regular teleconference meetings with modelers from Lawrence Livermore National Laboratory (LLNL), as well as other universities. These are working meetings that I have presented at many times, where I can get feedback and advice from experienced LLNL staff as well as offer advice.

Jeff Fein, University of Michigan (jrfein@umich.edu)

Degree: PhD, Nuclear Engineering and Radiological Sciences ❖ University Advisors: Professors James Holloway and R. Paul Drake ❖ SSAP: 2011-2016

Research Topic

Mitigation of hot electrons from laser-plasma instabilities in laser-produced x-ray sources

What are your research responsibilities?

For my graduate studies, I have been responsible for studying laser-plasma instabilities that are present in our laboratory astrophysics experiments. This study was motivated by the need to improve the soft x-ray backlighting techniques we use to image experiments studying radiative shocks and hydrodynamic instabilities. Laser plasma instabilities accelerate energetic or "hot electrons" that produce a background of hard x-rays on our detectors, contributing to degrading our radiographic data. From experiments, we observed a very large decrease in hot electron levels and hard x-ray backgrounds going from low- to high-Z laser-irradiated materials due to varying plasma conditions.

How did you benefit from the SSAP?

I benefitted from the SSAP both through direct funding during the first two years of graduate school, and through support and funding of the Center for Radiative Shock Hydrodynamics (CRASH) project that motivated my graduate research. The SSAP also provided me funding to attend and perform experiments critical to my thesis work, and to attend conferences to present my findings and meet other scientists.

Have you spent time at one of the national laboratories?

I performed experiments at Los Alamos National Laboratory (LANL) and at Lawrence Livermore National Laboratory (LLNL). At LANL, I used x-ray spectrometers to characterize laser-irradiated foils. I spent five weeks at LLNL conducting experiments on the transport of laser-produced MeV electrons. This gave me hands-on experience with many diagnostics, as well as with the unique laser systems themselves. I also had the opportunity to collaborate with several scientists there, whose input really helped make our experiment a success. Through all these experiences, I gained many skills relevant to performing experiments on a large laser facility, which can be a very challenging laboratory setting. Perhaps the most useful skill was the ability to make crucial decisions and adapt as we ran into unplanned issues with our experiments. Looking back, participating in these experiments at the national laboratories has been some of my best time spent doing research in graduate school!

Daniel Reese, University of Wisconsin, Madison (dtreese@wisc.edu)

Degree in Progress: PhD, Engineering Mechanics ❖ University Advisor: Dr. Riccardo Bonazza ❖ SSAP: 2012-Present

Research Topic

Experimental shock tube studies on the evolution of concentration and velocity-fluctuations in the Richtmyer-Meshkov instability

What are your research responsibilities?

My research responsibilities include all aspects of performing experimental research in the Wisconsin Shock Tube Laboratory (WiSTL), including the design, configuration, execution, and analysis of shock tube experiments. These experiments employ laser-based diagnostics such as planar laser-induced fluorescence (PLIF), correlation image velocimetry (CIV), and particle image velocimetry (PIV), as well as high-speed data acquisition to obtain flow information detailing the evolution of shock-accelerated inhomogeneous flows and the Richtmyer-Meshkov instability (RMI). I also write computer code used to process experimental data, and utilize the processed results to characterize the transition to turbulence and mixing in shock-accelerated interfaces.

How have you benefitted from the SSAP?

The SSAP has allowed me to carry out interesting and meaningful research during my time as a graduate student. In addition to supporting my studies at the University of Wisconsin, the SSAP has given me the opportunity to expand on my experimental research with computational experience though a summer internship at Lawrence Livermore National Laboratory (LLNL) as part of the High-Energy-Density Physics (HEDP) summer program. On top of all this, the SSAP has allowed me to attend a variety of conferences to present my research findings to the fluid dynamics community. As I complete my doctoral degree, the SSAP continues to support my experimental research and provides opportunities to share my work with fellow students and future colleagues.

Have you spent time at one of the national laboratories?

I spent the summer of 2014 at LLNL as part of the HEDP summer program. During this internship, I modeled experiments performed previously in the Wisconsin Shock Tube Laboratory using the high-order hydrodynamics code Miranda, and conducted a numerical investigation of three-dimensional (3D) effects on a 2D-dominated shocked mixing layer. That summer allowed me to broaden my experience as a researcher, giving me an exposure to computational techniques that greatly helped to expand my existing experimental expertise. My involvement in the HEDP program has opened my eyes to the abundance and variety of fascinating work being done at LLNL, and solidified my decision to work at a NNSA national laboratory full-time after obtaining my doctorate. I would highly recommend spending at least one summer at a national lab to all hard-working students lucky enough to be considering the opportunity.

Zachery Rehfuss, University of California, San Diego (zrehfuss@ucsd.edu)

Degree in Progress: BS Physics ❖ University Advisors: Dr. Brian Maple ❖ SSAP: 2015-Present

Research Topic:

Properties of novel d- and f- electron materials under high pressure and low temperature

What are your research responsibilities as an undergraduate in the lab?

As an undergraduate student in the Maple Group Laboratory, my research responsibility is to measure the physical phenomena that occur in novel *d*- and *f*- electron materials under extreme conditions such as high-pressure and low temperature. My current research project follows up work previously done in our laboratory involving phase transitions induced by magnetic field and chemical doping in $CeO_{1-x}F_xBiS_2$. I am furthering this work by investigating pressure-induced phase transitions in $CeO_{1-x}F_xBiS_2$ by measuring electrical resistivity using designer diamond anvil cells (dDacs) at pressures in the Mbar range and temperatures as low as 1K.

How have you benefitted from the SSAP?

The SSAP program has provided me with the opportunity to begin researching high pressure phenomena as an undergraduate under the guidance of Dr. Brian Maple. High-pressure work requires specialized equipment and training in order for experiments to have successful results. With funding from the program, I was able to travel to Lawrence Livermore National Laboratory (LLNL) to learn high-pressure techniques using dDacs and utilize those skills to do high-pressure measurements.

Has your experience working on this research influenced your future education / career plans?

Having the opportunity to conduct research as an undergraduate has solidified my desire to work towards a graduate degree in physics. In fact, I have been able to conduct research around the topic of high-pressure physics, which I intend to further study in graduate school. Working closely with Dr. Maple has allowed me to experience the lifestyle of a research physicist, which has encouraged me to pursue a career as a researcher at either a university or a national laboratory.

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

The SSAP has given me the opportunity to collaborate with researchers from LLNL. The program not only allowed me to collaborate with coworkers from LLNL but also allowed me to travel to LLNL to acquire the skillset necessary to carry out electrical resistivity measurements under extremely high pressure using dDACS.

Raspberry Simpson, Massachusetts Institute of Technology (razzy@mit.edu)

Degree: PhD, Nuclear Engineering ❖ University Advisor: Dr. Richard Petrasso ❖ SSAP: 2016-Present

Research Topic

Charged particle diagnostics for inertial confinement fusion

What are your research responsibilities?

Currently, I am working on developing a new diagnostic for the National Ignition Facility (NIF) called the Thomson Parabola Charge Particle Spectrometer (TP-CPS). TP-CPS will combine design elements of electric and magnetic spectrometers with parallel electric and magnetic fields that can discriminate particles based on their charge-to-mass ratio. The TP-CPS's ability to measure various particles with a broad energy range (~0.5-100 MeV) will be crucial for experiments involving acceleration of fast ions, such as experiments with the new Advanced Radiographic Capability (ARC), and for experiments studying plasmas relevant to stellar nucleosynthesis, stopping power, collisionless shocks, and other basic high energy density plasma physics phenomena. In addition to this effort, I am also working on experiments to investigate the role of multi-ion species effects in shock-driven inertial confinement fusion (ICF) implosions at the Omega Laser Facility at the University of Rochester Laboratory for Laser Energetics.

What do you want students considering the SSAP to know?

Stewardship science is interdisciplinary, allowing my involvement with many cross-cutting areas of research ranging from fundamental plasma physics to material science. In addition, the SSAP has enabled me to get very involved with the broader stewardship science community by giving me the unique opportunity to collaborate with many scientists at DOE/NNSA national laboratories like Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory. Many of these scientist have been able to provide me with crucial help, support, and feedback in my research.

Have you spent time at one of the national laboratories?

Before joining Dr. Richard Petrasso's group at MIT, I worked at LANL for two years as a post-Baccalaureate research student helping to develop neutron imaging diagnostics for the NIF. I believe this experience really helped me to gain confidence as a researcher and inspired me to continue this line of research at the graduate level. As a student at MIT, I am excited every day to continue work in ICF and fusion energy in general.

David Walter, Rutgers University (dwalter@physics.rutgers.edu)

Degree: PhD, Physics ❖ University Advisor: Dr. Jolie Cizewski ❖ SSAP: 2013-Present

Research Topic

Nuclear structure of exotic, neutron-rich nuclei and single particle transfer reactions

What are your research responsibilities?

I am responsible for the analysis of a (d,p) reaction that was measured at the National Superconducting Cyclotron Laboratory (NSCL) with stable ^{86}Kr beams at 35 MeV/A and the Oak Ridge Rutgers University Barrel Array of position-sensitive silicon strip detectors, developed with Stewardship Science Academic Alliance support. This neutron transfer measurement is used as a proof of principle to test a combined method for extracting spectroscopic information from neutron-rich nuclei near the r-process path of nucleosynthesis. Due to the promising results of the ^{86}Kr(d,p)^{87}Kr measurement, I am also the principal investigator for an approved experiment to measure the radioactive ion beam ^{84}Se(d,p)^{85}Se reaction at the NSCL. I lead the efforts in planning and testing the setup, and will take the lead in analyzing the data from the experiment to be completed in 2017.

How have you benefitted from the SSAP?

The SSAP has provided me with many opportunities to travel to workshops at Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory, and also take part in many experiments and conferences. Participating in experiments has helped me to learn different experimental measurement techniques for transfer reactions, beta-delayed neutrons, and also neutron-induced fission. While travelling to conferences, I have been able to share my own work as well as meet many other scientists from across the United States and the world. Discussions with scientists from NNSA national laboratories and universities has proven to be very beneficial in my own research, as well as allowed me to make connections for my future career.

Have you spent time at one of the national laboratories?

I am fortunate to be in residence at Oak Ridge National Laboratory, where I conduct all of my graduate research. Working side by side with postdoctoral researchers and staff scientists has allowed me to contribute to many other projects, including the development of a new liquid scintillator array used for neutron detection. Through the SSAP, I have participated in experiments at Argonne National Laboratory, the NSCL, and also the University of Notre Dame. In the winter of 2016, I had the opportunity to spend two months at LANL to help with measurements of neutron-induced fission cross sections of U and Pu isotopes. I worked at the Los Alamos Neutron Science Center (LANSCE) where I met many remarkable scientists, and also experienced the day-to-day operations during a typical LANSCE run cycle. My involvement in the variety of experiments and detector systems ranging from nuclear structure to fission has provided me with great experience for a future career in many areas of nuclear physics.

Blake Wiggins, Indiana University (brywiggi@indiana.edu)

Degree: PhD, Chemistry ❖ University Advisor: Dr. Romualdo T. deSouza ❖ SSAP: 2013-Present

Research Topic

Development of a high-resolution position sensitive microchannel plate detector

What are your research responsibilities?

My primary responsibility is detector and electronics development, which includes design, construction, and testing for a novel microchannel plate-based imaging detector. I work in the low energy nuclear chemistry group with Dr. Romualdo deSouza and typically am characterizing the detector and associated electronics to optimize its spatial resolution in two dimensions. I am engaged in thinking at a fundamental level about the underlying physics and ramifications on the detector design and signal processing. This new detector will soon be used to make neutron radiographic measurements at the Low Energy Neutron Source at Indiana University.

How have you benefitted from the SSAP?

SSAP funding has been critical in the development of this new imaging detector. The program also facilitates attending conferences, which have led to an invaluable number of discussions with other researchers. For example, at the annual SSAP symposium, I was able to discuss positron emission tomography, a possible application for my detector, with an expert in the field. In general, the program has expanded my breath of knowledge into various fields, especially in regards to stockpile stewardship.

What do you want students considering the SSAP to know?

The SSAP supports universities that conduct fundamental science and technology research of relevance to stockpile stewardship. First and foremost, the program is investing in training the next generation of scientists. The program also facilitates exposure and networking opportunities to national laboratories through visibility to DOE/NNSA scientific activities. Overall, this program is a great platform for development of scientists by providing intellectual exchange and collaboration, especially in conjunction with the NNSA national laboratories.

UF UNIVERSITY of FLORIDA

ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

UNIVERSITY OF
NOTRE DAME

Stanford
University

ATM
TEXAS A&M
UNIVERSITY

THE
UNIVERSITY
OF UTAH

Predictive Science Academic Alliance Program

As a result of a Funding Opportunity Announcement (FOA) released in 2012 by the Advanced Simulation and Computing (ASC) Program in the Office of Defense Programs within the Department of Energy's National Nuclear Security Administration (NNSA), six new centers of excellence were established. Six universities operate research centers focused on demonstrating predictive science in a high-performance-computing environment, as part of the NNSA's Predictive Science Academic Alliance Program II (PSAAP II). Three of the sites are Multidisciplinary Simulation Centers (MSCs) and three are Single-Discipline Centers (SDCs) funded at approximately $4M and $2M, respectively, per year for five years. Each Center is using a multi-scale and multi-physics 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. Due to the complexity of the applications, predictive science can only be done on the most powerful computers available. In order to prepare for the next round of advanced systems whose architectures will present issues of usability, the Centers are conducting research in computer science that can be expected to contribute to the effective usability of these new systems. The six Centers are listed below.

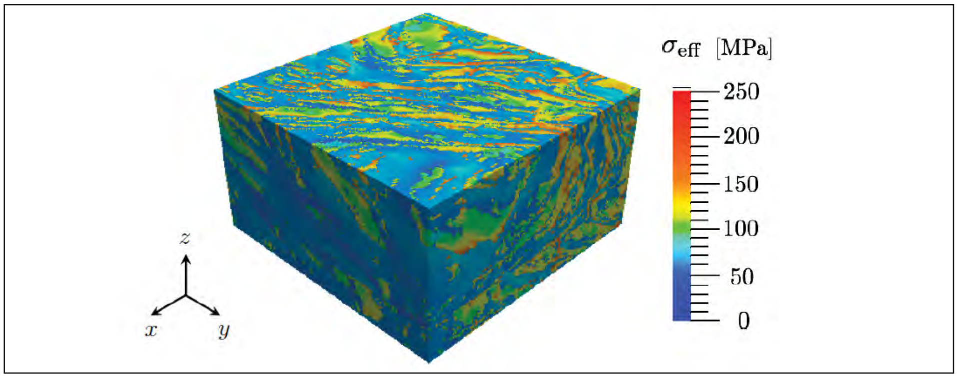

Figure 1. At the University of Notre Dame, a heterogeneous material system reconstructed from micro-tomography was simulated to verify a newly developed numerical method to predict mechanical behavior under different loading conditions using crystal plasticity constitutive equations. Forty million nonlinear equations are solved together with 1 billion ODEs for 13 million finite elements.

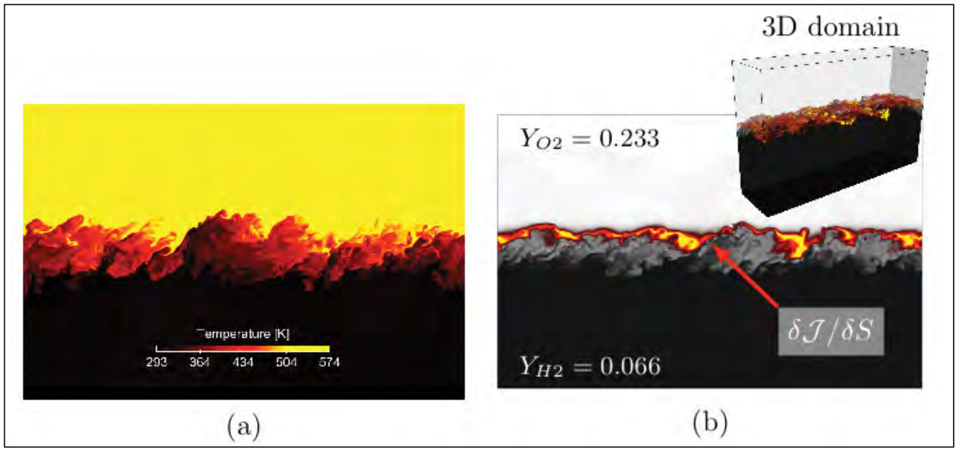

Figure 2. The Center at the University of Illinois simulates free-shear-flow turbulence to isolate the effect of turbulence on ignition sensitivity. Figure (a) shows that the compressible reactive shear layer has developed to exhibit a broad range of spatial scales. This simulation used 300 million grid points to discretize the domain. The solution was integrated in time by 72,000 time steps in 18 hours using 32,000 central processing units. Figure (b) shows the sensitivity (δJ/δS) of the space-time integrated heat release (J) with respect to a thermal source (S) added to evolution of the total non-chemical energy equation.

- University of Florida
  Compressible multiphase turbulence resulting from explosions such as a volcanic eruption.
- University of Illinois
  Plasma coupled combustion in ignition of fuel in, for example, automobile engines.
- University of Notre Dame
  The impact of shocks on heterogeneous materials.
- Stanford University
  The effect of radiation on particle motion in a turbulent airflow in solar thermal receivers with applications in energy production.
- Texas A&M University
  Radiation transport in nuclear reactor design and astrophysics.
- University of Utah
  The simulation of large clean-coal boilers leading to clean generation of electricity.

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 third year and, to date, nearly 100 students have taken advantage of the opportunity. In many cases, the student continues interacting with their laboratory mentor after returning to their university, and some of the students have returned for a second internship. These internships provide the national 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 at least 12 students after they completed their PhD.

In the text that follows, six students, one from each Center, discuss their experiences with PSAAP II.

David Zwick, University of Florida (dpzwick@gmail.com)

Degree in Progress: PhD, Mechanical Engineering ❖ University Advisor: Dr. S. Balachandar ❖ PSAAP: 2015-2016

Research Topic

Higher-order multiphase simulation with particles

While I have always been captivated by fluid flow, my final graduate school choice was a tough decision as there were many exceptional schools where I could pursue my interests. The PSAAP II-funded Center for Compressible Multiphase Turbulence (CCMT) at the University of Florida (UF) was the deciding factor for me when I made my final decision to attend UF. When I initially toured the CCMT, I was immensely impressed with the high quality research, expert staff, and exemplary organization found there. Now, having worked at the CCMT for over a year, I have not been disappointed.

Figure 1. Explosive dispersal of 114-mm Al particles.

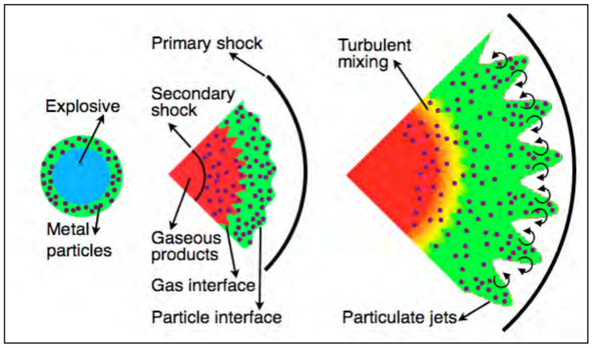

Figure 2. Computational domain.

> *"The PSAAP II-funded Center for Compressible Multiphase Turbulence (CCMT) at the University of Florida (UF) was the deciding factor for me when I made my final decision to attend UF. When I initially toured the CCMT, I was immensely impressed with the high quality research, expert staff, and exemplary organization found there. Now, having worked at the CCMT for over a year, I have not been disappointed."*

After officially arriving at the CCMT, I quickly became acquainted with the goals, methodology, and broader impacts of the ongoing research. The overarching goal of the CCMT is to extend the current predictive abilities of simulation through study of our chosen model problem, which is the explosive dispersal of solid particles (see Figures 1 and 2). This aligns well with my research interests, which is focused on the high-accuracy treatment of particulate phases in multiphase simulations. In pursuit of this common goal, I soon became immersed in the interdisciplinary environment at the CCMT consisting of engineers, mathematicians, and computer scientists. Based on my research interests, I would classify myself as an engineer; however, the expertise of computer scientists and applied mathematicians has significantly aided in my research. As an example, at the CCMT, we have been developing code called CMT-nek that will solve the three-dimensional conservation equations for a compressible multiphase fluid flow with turbulence. Over the past year, I have added a significant amount of code to solve the governing equations for particulate phases, which represent the dispersed solid particles of the CCMT's model problem. However, in order to accurately study the physics of the problem, an enormous number of particles needs to be used. Due to the large number of particles, any code that I write must be scalable to hundreds of thousands of processors on modern supercomputers. This aspect has led me to interact with many computer science professors and students so that I can efficiently implement physically meaningful simulations that utilize the supercomputing resources available at the weapons national laboratories.

This summer, I gained further understanding and expertise as an intern at Sandia National Laboratories (SNL) as a part of the PSAAP requirements. I worked with my mentor there, Dr. Kevin Ruggirello, to implement particle capabilities in the shock-physics code CTH. My summer experience at SNL was extremely positive and greatly assisted in my research and professional goals. In my time there, I implemented a coupling algorithm for particulate phases to influence the surrounding fluid. This was beneficial for me because this coupling is only required to match the accuracy of the fluid, which is of lower-order in CTH. However, in CMT-nek, this is of higher-order, which poses challenges in developing numerical methods for effectively doing this. My work with CTH was a good starting point that allowed me to understand essential aspects of particle-fluid coupling in the simpler lower-order context. On top of this, I was thoroughly impressed by the friendliness and willingness of SNL staff to assist me when I had questions or concerns. I am very grateful for all those associated with the PSAAP who have guided me and I am eager to continue the research and relationships facilitated by the program.

Andrew Reisner, University of illinois at Urbana-Champaign (areisne2@illinois.edu)

Degree in Progress: PhD, Computer Science ❖ University Advisor: Luke Olson ❖ PSAAP: 2014-Present

Research Topic

Scalable linear solvers

The efficient solution of sparse, linear systems is a significant computational challenge in many applications, including the electric field calculations in our predictive simulations through the Center for the Exascale Simulation of Plasma-Coupled Combustion at the University of Illinois at Urbana-Champaign. The focus of my work is on the scalable performance of multilevel solvers, where modern architectures for high-performance computing systems continue to challenge parallel scalability. By taking advantage of structure, notable performance advantages such as direct memory access and bounded complexity in the multigrid cycle can be achieved. To this end, my research is on the parallel development and performance of black box multigrid (BoxMG), a robust variational solver on structured grids. The potential of this framework is promising as we look to extend the multilevel methodology and exploit the structure in more general, multi-block settings. The project is supervised by Luke Olson and William Gropp at the University of Illinois at Urbana-Champaign, in collaboration with David Moulton at Los Alamos National Laboratory, where I have spent the last two summers designing and developing the parallel components of the algorithm.

One common hindrance to parallel scalability is coarse-grid problems. When problems become coarser, the computation to communication ratio becomes less desirable. This is especially problematic on modern machines with large cost disparities between data movement and floating-point operations. Initial distributed implementations of BoxMG gathered the coarse-grid problem to a single core, which is beneficial when the cost of serial cycling offsets the cost of continued parallel coarsening. On current machines, this approach limits weak scalability due to the growth in the coarse-grid with the number of processors. To extend the scalability of this approach, I have developed a redistribution process for coarse problems through incremental agglomeration. To robustly choose an efficient agglomeration sequence, my approach utilizes a predictive performance model to guide the coarse grid redistribution.

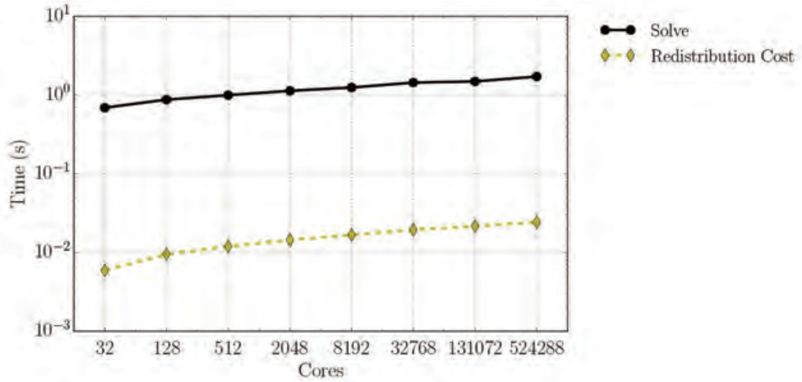

Figure 1. Weak scaling of BoxMG solve on Mira with local problem size: 568 x 71.

> *“The potential of this framework is promising as we look to extend the multilevel methodology and exploit the structure in more general, multi-block settings. The project is supervised by Luke Olson and William Gropp at the University of Illinois at Urbana-Champaign, in collaboration with David Moulton at Los Alamos National Laboratory, where I have spent the last two summers designing and developing the parallel components of the algorithm.”*

The coarse grid redistribution algorithm is divided into two stages: redistribution enumeration and redistribution search. In the first stage, potential agglomerated processor grids are enumerated by beginning with one coarse task and refining greedily by dimension with respect to the local problem size. This effectively controls the size of the search space while permitting redundant coarse-grid cycling and maintaining a tensor product processor grid structure. The recursive application of this approach generates a global search space. Our predictive performance model is then used to define a metric on this search space and an optimal redistribution path is chosen. Figure 1 shows weak scaling of our algorithm on Mira, an IBM BG/Q at Argonne National Laboratory. These results confirm favorable weak scaling behavior on over 500,000 cores.

In the future, I plan to work on extending robust variational multigrid on structured grids to multi-mesh and multi-block settings. This would enable exploiting local structure to gain the performance advantages of structured computation that are increasingly important on modern architectures for a range of applications. Addressing coarse-grid parallel scalability limitations in BoxMG is an important step towards a scalable, high-performance solver that can be used in the development of a structure-exploiting framework.

Cale Harnish, University of Notre Dame (charnish@nd.edu)

Degree in Progress: PhD, Aerospace & Mechanical Engineering ❖ University Advisor: Dr. Karel Matouš ❖ PSAAP: 2014-2016

Research Topic

Computational modeling of high-strain rate response and instabilities of heterogeneous solids

The Predictive Science Academic Alliance Program II (PSAAP II) has aided in the creation of a highly collaborative and interdisciplinary research environment at the University of Notre Dame. At the Center for Shock Wave-processing of Advanced Reactive Materials (C-SWARM), I am immersed in a research culture that is focused on data-driven computational materials science that is verified, validated, with quantified uncertainties. As a member of this PSAAP II Center of Excellence, I am working with Dr. Karel Matouš, the director of C-SWARM, to develop a novel numerical method that can solve partial differential equations whose solutions contain a wide range of spatial scales. Our exciting research will facilitate the modeling of high-strain rate dynamics by reducing the large computational requirements inherent in many traditional numerical methods and will utilize future exascale computing platforms.

In the summer of 2015, I had the opportunity to experience the PSAAP summer internship program with the NNSA national laboratories. I was invited to work with Dr. Daniel Livescu at Los Alamos National Laboratory (LANL). I was welcomed into the Computational Physics and Methods group within the Computer, Computational, and Statistical Sciences division, and had the opportunity to attend several seminars and laboratory tours. Working with Dr. Livescu over the summer, I learned the fundamentals of wavelet basis functions and how they may be used to solve partial differential equations. The PSAAP summer internship program exposed me to the many alternatives to academia offered by the national laboratories, allowed me to network with other graduate students in my field, and helped me cultivate a strong connection between LANL and the University of Notre Dame.

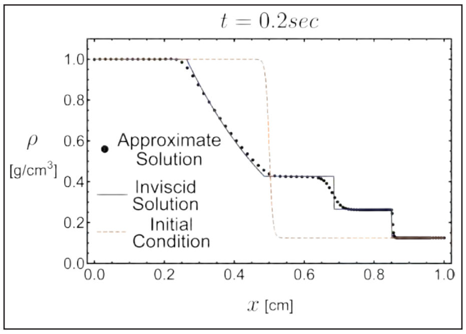

Figure 1. The density field for a viscous fluid in the Sod shock tube problem at 0.2 seconds. The zero viscosity solution (solid line) and the initial condition (dashed line) are shown for comparison. Our algorithm well resolves the shock wave, the contact surface, and the rarefaction wave.

Upon my return to University of Notre Dame, interactions continued between Dr. Livescu, Dr. Matouš, and myself. Together, we proposed a collaborative PhD research thesis for adaptive multiscale modeling of high-strain rate dynamics and instabilities in heterogeneous solids. As part of this collaboration, Dr. Livescu agreed to serve on my PhD committee. Dr. Matouš and I regularly videoconference with Dr. Livescu on our research progress and I've been invited to return to LANL each summer. I made my second visit to LANL in the summer of 2016 where I finalized the theory and one-dimensional (1D) implementation of our dynamically adaptive, wavelet-based, pseudo-spectral method for solving nonlinear partial differential equations.

> *"As a member of this PSAAP II Center of Excellence, I am working with Dr. Karel Matouš, the director of C-SWARM, to develop a novel numerical method that can solve partial differential equations whose solutions contain a wide range of spatial scales. Our exciting research will facilitate the modeling of high-strain rate dynamics by reducing the large computational requirements inherent in many traditional numerical methods and will utilize future exascale computing platforms."*

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Our novel algorithm constructs a dynamically adaptive computational grid by representing fields and operators in terms of wavelet basis functions. The multi-resolution nature of wavelets notably reduces the memory cost associated with solving large problems and allows computations to be calculated only in regions where sharp transitions occur. We have constructed our algorithm to solve problems on finite domains and have obtained accurate solutions with explicit error control, high data compression, and no spurious numerical oscillations. We have verified our method on a variety of 1D shock problems such as the Sod shock tube, which has an analytical solution for zero viscosity fluids. The figure shows the density field that we have calculated for a viscous fluid. It can be seen that the shock wave in the far right of the image is well resolved and that our solver adds points to the computational grid only in the locations where structures develop. As our research progresses, this innovative algorithm will be parallelized, extended to N-dimensional problems, applied to problems of high-strain rate dynamics, and a variety of other engineering applications.

Jeremy Horwitz, Stanford University (horwitz1@stanford.edu)

Degree in Progress: PhD, Mechanical Engineering ❖ University Advisor: Professor Ali Mani ❖ PSAAP: 2014-Present

Research Topic

Particle-laden turbulent flows, point-particle modeling, momentum and energy coupling, verification and validation

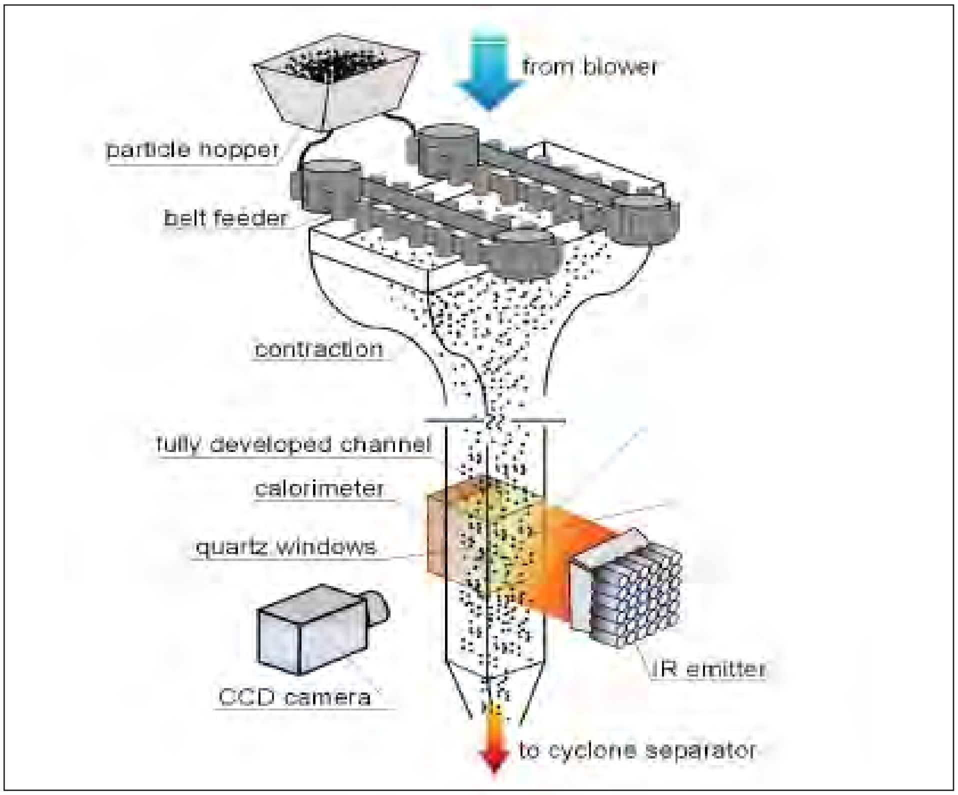

Figure 1. Schematic of Stanford University Focus Problem.

My work in the PSAAP II program has focused on developing verifiable models that accurately predict fluid systems laden with a dispersed solid phase. Such systems include volcanic ash transport and sand dunes interactions with the atmospheric boundary layer. In the PSAAP II program, we are investigating alternative means of power conversion whereby opaque small particles absorb solar radiation and then convect their internal energy volumetrically to turbulent air (see Figure 1). The heated air can then be used to extract work as is done, for instance, in vapor power plants. While considerable work has been done in this area, the physics of how small particles interact with turbulence is still not fully understood. We have adopted a standard approach which solves the continuum fluid equations at fixed (Eulerian) locations and tracks individual point-particles in their respective (Lagrangian) frames. In this methodology, the flow is not resolved on the scale of the particles, so the coupling between particles and fluid comes from an assumed drag model which takes into account physical parameters in the system (for instance particle size, fluid viscosity, slip velocity between particles and fluid, etc.).

Simulation models require verification and validation. In verification, we ask, "with this assumed model, how do I, as the user, know that I have implemented the model correctly?" During validation, we ask, "how predictive is the verifiable model?" My work has largely focused on these two questions. We showed early on in the program that two-way coupled simulations where particles and fluid exchange momentum and energy are not verifiable even under the conditions where a Stokesian particle settles under gravity in an otherwise stationary fluid. The major issue is that drag laws demand the undisturbed fluid velocity at the location of the particle, but only the disturbed fluid velocity, that which can be calculated by interpolation from the surrounding fluid points, is directly available in the simulation. We developed a procedure for estimating the undisturbed velocity and showed that this procedure was consistent with accurate settling velocities. More recently, we compared our method to a fully resolved simulation for the case of decaying particle-laden turbulence. When the appropriate drag law was applied with the undisturbed fluid velocity, our method agreed well with the higher resolution simulations.

During the winter of 2016, I had the pleasure of working with a great team at Los Alamos National Laboratory (LANL) led by Dr. John Schwarzkopf, along with Dr. Daniel Livescu, and Dr. Peter Brady. This was my second time working at LANL, the previous time being a summer internship where I was mentored by Dr. Schwarzkopf during the summer of 2013. In 2016, I ended up working on two projects. The first was the application of fully resolved particles to particle-turbulence interaction. The goal was to understand fundamentally how a single particle or array of particles serves to modify turbulence. During this project, I gained a lot of insight about particulate physics which was beneficial towards my modeling project at Stanford. In the second project, I worked on an extension to the research I had done during the summer of 2013 by developing the transport equations for mean thermal energy and turbulent heat flux with the addition of particle effects. This work lays out the exact unclosed terms in the thermal transport equations which will help in understanding of fundamental physics as well as for model development of particle-laden flows with heat transfer.

Kelli Humbird, Texas A&M University (khumbird@tamu.edu)
Degree in Progress: PhD, Nuclear Engineering ❖ University Advisor: Dr. Ryan McClarren ❖ PSAAP: 2016

Research Topic

Surrogate models for identifying robust, high-yield inertial confinement fusion implosions

I received my Master's Degree in nuclear engineering from Texas A&M in May 2016, and plan to continue on to a PhD with my research advisor, Dr. Ryan McClarren. Prior to beginning my dissertation work, I was given the opportunity to spend the summer at Lawrence Livermore National Laboratory (LLNL) as a high energy density physics intern with Dr. Luc Peterson.

During the Phase I Trinity Open Science Campaign in 2016, the Inertial Confinement Fusion (ICF) program's Ensembles Simulations Team at LLNL created the largest collection of two-dimensional (2D) ICF implosion simulations. The approximately 60,000 simulations consumed 39 million central processing unit-hours and generated 5 PB of raw data (see Figure 1). The database involved a 9D parameter scan of time-varying drive asymmetries, drive amplitudes, and capsule gas fill densities. My task for the summer was to construct surrogate models, which are approximations to the true response surface, and use them to search for robust, high-yield implosions. Multiple machine learning methods were tested for the construction of the surrogates; the complicated topology of the response surface challenged even the most robust algorithms. The model that is best suited for the ICF data is the random forest regressor, which uses a collection of decision trees built on bootstrapped samples from the training data to make predictions. Surrogates are constructed for multiple quantities of interest; in particular, the model for the yield has a predictive accuracy of 94% when trained on 80% of the data.

A Nelder-Mead optimization algorithm and the surrogates are used to identify the implosion in design space that has high yield and is insensitive to perturbations in the input parameters. The optimal implosion is ovoid in shape and is predicted to have higher yield and be more robust than a spherical implosion, which is traditionally accepted to be ideal. Additional simulations confirm the surrogate predictions, and demonstrate that the ovoids are less sensitive to drive asymmetries and perturbations (such as deuterium-tritium ice roughness, or the presence of the tent that holds the capsule in place) than spherical implosions. The simulations provide physical insight into why the ovoid implosions perform well: A time-varying drive asymmetry compresses the capsule in a "sausage" shape early in time, creating axial jets that flow out the top and bottom of the capsule; this is followed up by a "pancake" compression, which prevents these jets from escaping. Countering propagating, coaxial vortex rings are formed, with the flow going into the central hotspot at the equator and out at the poles. The cold dense shell on the equator accretes into the center, fueling the hotspot without distorting its shape. Further investigation into the robustness of the ovoid implosions when exposed to all sources of yield degradation are needed in order to determine how they compare to spherical implosions under realistic conditions.

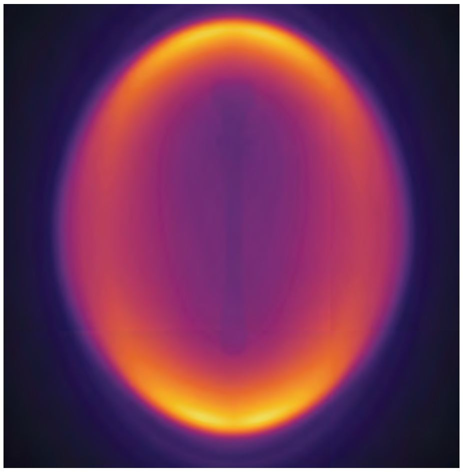

Figure 1. Simulated density at the time of maximum energy production for a robust ovoid inertial confinement fusion (ICF) implosion, the parameters for which were chosen by a machine learning model trained on the largest ICF simulation database ever created (5 PB; 60,000 simulations).

> *"The discovery of this family of implosions is a clear illustration of the power of machine learning in furthering our understanding of complicated physical systems. After such an exciting and promising summer, we feel that the database has much more to teach us about ICF implosions, and I was invited to complete my PhD research at LLNL."*

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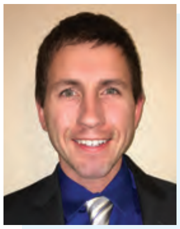
The discovery of this family of implosions is a clear illustration of the power of machine learning in furthering our understanding of complicated physical systems. After such an exciting and promising summer, we feel that the database has much more to teach us about ICF implosions, and I was invited to complete my PhD research at LLNL. My dissertation will be focused on Bayesian hierarchical uncertainty quantification for model validation and extrapolation into regimes that are not currently achievable on the National Ignition Facility.

Benjamin Schroeder, University of Utah (bbschro@sandia.gov)

Degree: PhD, Chemical Engineering ❖ University Advisor: Sean Smith ❖ PSAAP: 2014-2015

Research Topic



Validation and uncertainty quantification for large-scale computing and reduced-order modeling

Through the PSAAP II program, I was afforded the opportunity to explore validation and uncertainty quantification theory and methods, and apply this knowledge to large-scale, physics-based simulations to aid real world decision-making processes. The PSAAP II program allowed my research center, the Carbon-Capture Multidisciplinary Simulation Center, to create large-scale simulations of full-scale, next-generation coal boilers that could produce energy more efficiently than technologies currently employed (see Figure 1). It was upon these simulations that I was able to apply uncertainty quantification methods to produce simulation predictions with uncertainty estimates and quantified understanding of the simulation's predictivity through validation comparisons with experimental data.

As part of the PSAAP II program, I participated in a summer internship at Sandia National Laboratories (SNL), where I joined a group focused on verification, validation, uncertainty quantification and credible processes for large-scale simulations of engineering applications. During my internship, I interacted with a variety of experts in my field of study and was able to diversify my worldview on my research topical area. I began my summer internship investigating Bayesian statistical methods of approaching model form uncertainty, or the uncertainty attributed to a model's inadequacies, but came to understand that these methods were part of a bigger movement to solve what is known as the uncertainty rollup problem. The objective of the uncertainty rollup problem is to use information gained through activities including parameter calibration, sensitivities analysis, and model validation to make better-informed predictions in regions without experimental data.

> *"As part of the PSAAP II program, I participated in a summer internship at Sandia National Laboratories, where I joined a group focused on verification, validation, uncertainty quantification and credible processes for large-scale simulations of engineering applications. During my internship I interacted with a variety of experts in my field of study and was able to diversify my worldview on my research topical area."*

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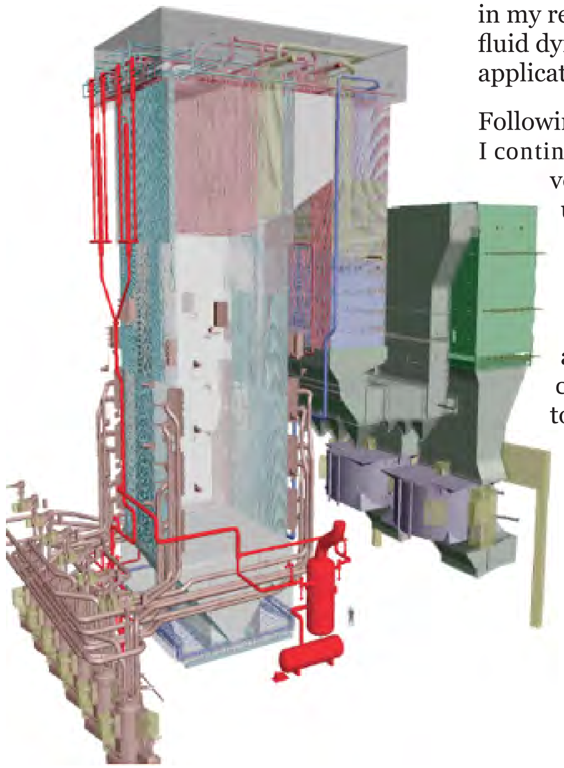

Figure 1. High-efficiency advanced ultra-supercritical oxy-coal tangentially-fired power boiler.

My exposure to this community of researchers directly impacted my ultimate dissertation topic, the construction of reduced-order models for large-scale physics simulation. A major idea presented in my dissertation was that tools from the verification, validation, and uncertainty quantification field can aid in the creation of physics models of reduced complexity, specifically scoped to capture physical phenomena of interest at scales appropriate to large-scale computing of full system applications. These models of reduced complexity need to propagate uncertainty in a fashion similar to the equivalent models of full complexity, but at a realizable computational cost. Combining physics modeling with parameter calibration, uncertainty quantification, and model validation techniques allowed me to create a reduced-order coal-particle devolatilization model that was able to recreate the predominant uncertainty found in a high fidelity model. This reduced-order coal-particle devolatilization model was implemented in my research center's computational fluid dynamics code and used to make application-scale coal boiler predictions.

Following my dissertation defense, I continued my research in the verification, validation, and uncertainty quantification field as a Postdoctoral Appointee at SNL with the group with whom I completed my internship. Since then, I have converted to a full-time staff member, but continue my research on the same topical areas: model validation, uncertainty quantification, model form error and the uncertainty rollup problem, all applied to large-scale simulations of engineering applications.

Stewardship Science Graduate Fellowship

Alex B. Zylstra, Los Alamos National Laboratory (zylstra@lanl.gov)

Degree: PhD, Physics ❖ University/Advisor: Massachusetts Institute of Technology/Dr. Richard Petrasso ❖ SSAP: 2009-2015

I did my graduate work at the Massachusetts Institute of Technology (MIT), supported by the Stewardship Science Academic Programs and by the Stewardship Science Graduate Fellowship (SSGF) program. I worked in Dr. Richard Petrasso's High-Energy-Density Physics (HEDP) Division and inertial confinement fusion (ICF) group. My thesis work included three projects: proton spectroscopy on the National Ignition Facility (NIF), charged-particle stopping power measurements, and studies of fusion reactions relevant for nuclear astrophysics.

In the first project, I applied proton spectroscopy techniques developed by the MIT group to studying implosions on the NIF. While the ultimate goal of NIF is to ignite a compressed deuterium-tritium (DT) plasma, many surrogate experiments are conducted using deuterium and helium-3 (D^{3}He) fuel instead. The D^{3}He reaction produces an energetic proton, which I used to study several aspects of the implosion dynamics, including the shock dynamics[1] and in-flight implosion asymmetries.[2]

Using the same proton spectroscopy techniques, I also developed a new experimental technique for measuring the stopping power, or energy loss rate, of energetic charged plasmas. The stopping power is well known in classical plasmas, but in many HEDP regimes, classical theories break down, requiring more advanced techniques that had not been experimentally tested. I measured the stopping power in warm-dense-matter beryllium, finding good agreement with the best theoretical models.[3]

Thirdly, I studied nuclear reactions relevant to astrophysics. Rather than filling an ICF target with typical fusion fuels, such as DT or D^{3}He, we can use a different fuel that contains reactants for a process relevant to nuclear astrophysics. One such reaction is the fusion of T and ^{3}He, which can produce lithium-6 (^{6}Li) and an energetic γ ray. This reaction is potentially important during big-bang nucleosynthesis (BBN), a process that produced some light elements a few minutes after the big bang. Astronomers have observed anomalously-high levels of ^{6}Li in primordial materials, which cannot be explained using standard BBN theory. Several researchers had hypothesized that the T^{3}He reaction might explain the levels of ^{6}Li. Using ICF implosions, I took the first measurement of the cross section for this reaction in the energy range relevant to BBN (see Figure 1), finding it to be too low to explain the ^{6}Li abundances.[4] While a final resolution is still elusive, this data suggests that BBN nuclear physics is not the solution.

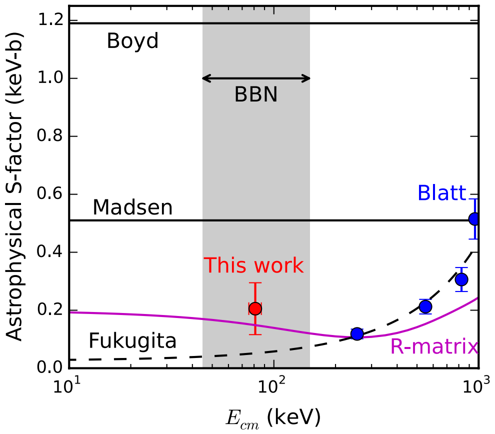

Figure 1. Astrophysical S-factor, related to the reaction cross section, for T+3He fusion. This measurement (red) is the first in the energy range relevant to BBN (grey bar). New theory (magenta curve) is being used to connect to high-energy accelerator data (blue). Our data also show that values used in BBN codes (black curves) are inaccurate.

In addition to funding my graduate work, the SSAP and SSGF programs were extremely beneficial in positioning me for a career at the NNSA national laboratories by helping to develop collaborations and meet laboratory researchers at the annual meetings. After defending my dissertation in 2015, I accepted a Reines Distinguished Fellowship at Los Alamos National Laboratory.

My postdoctoral fellowship allowed me to extend some of my thesis work while also becoming involved in the programmatic work. I have a continuing collaboration with the MIT group on stopping power, developing a new platform at NIF, and nuclear astrophysics, by applying the γ-ray diagnostics to new reactions. In addition to these basic science topics, I am working on LANL ICF programmatic experiments on mix in ICF implosions and reduced-compression implosion physics experiments.[5] I recently converted to a staff scientist position at LANL, with my role evolving to include working for several projects to execute experiments on the NIF.

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[2] A.B. Zylstra et al., Phys. Plasmas 22, 056301, 2015.

[3] A.B. Zylstra et al., Phys. Rev. Lett. 114, 215002, 2015.

[4] A.B. Zylstra et al., Phys. Rev. Lett. 117, 035002, 2016.

[5] R.E. Olson et al., Phys. Rev. Lett. 117, 245001, 2016.

Sarah Palaich Heffern, University of California, Los Angeles (palaich@gmail.com)

Degree: PhD, Geochemistry ❖ University Advisor: Professor Abby Kavner ❖ SSGF Program: 2013-2016

Research Topic

Carbon in the deep earth

What are your research responsibilities?

While in graduate school, I spearheaded several projects involving carbon in the deep earth. I brought together scientists from the Spallation Neutron Source at Pressure (SNAP) beamline, Spallation Neutron Source, Oak Ridge National Laboratory with a group from UCLA, supported by the Deep Carbon Observatory, to conduct the first neutron diffraction experiments in a diamond anvil cell at high temperature (up to 625 K). These experiments were successful and also produced much needed additional data on the intermediate phases of CO_2. I am especially proud of this collaboration, as I built it one phone call at a time and can watch it continue after my time at UCLA.

I also collaborated with Professor Marco Merlini at the University of Milan, with whom I conducted research on several carbonates using single crystal x-ray diffraction at the European Synchrotron Radiation Source.

How have you benefitted from the SSGF Program?

The most important thing the SSGF gave me is freedom. It gave me the freedom to forge new research projects that my advisors would not necessarily have been able to fund me on independently. This freedom allowed me to explore new research opportunities and to collaborate with researchers across the globe.

Have you spent time at one of the national laboratories?

I've spent time at numerous DOE/NNSA national laboratories (Argonne, Berkley, Los Alamos, and Oak Ridge), but the time spent in my practicum at Los Alamos National Laboratory was the most useful. My time there was a fantastic experience that allowed me to explore new branches of geology and forge new collaborations and connections. I learned more about the workings of a national laboratory, but the most important part of my experience centered around the people I worked with. My colleagues were not just interested in me as a scientist; they were interested in me as a person. I had meetings with the head of my department about the state of science education and how important it is to commit to the improvement of science education in this country. I found people who wanted me to succeed outside of academia, industry, or the laboratories. They were proud of my efforts to become a teacher and they gave me opportunities to join national geologic organizations to make a difference from within the field. This support would never have been possible without the practicum experience offered by the SSGF program.

Io Kleiser, California Institute of Technology (ikleiser@caltech.edu)

Degree in Progress: PhD, Astrophysics ❖ University Advisor: Professor Sterl Phinney, collaboration with Daniel Kasen ❖ SSGF Program : 2012-2016

Research Topic

Unusual explosions of massive stars

What are your research responsibilities?

I run simulations using a variety of codes to follow the birth, evolution, and death of massive stars and understand what they look like when they explode. Throughout its life, the structure of a star may change significantly; mass can be lost due to radiation-driven winds for very luminous stars, or a stellar companion may gravitationally attract and remove mass from the outer edge of the star. Various stages of nuclear burning can cause the star to heat and puff up or even eject material. All of these changes have an effect on the observable signatures of the supernova. Using an open-source stellar evolution code (MESA), my own hydrodynamics code, and a radiation transport code (SEDONA), I can do end-to-end calculations of a star's life and death, then predict what each supernova from each star with its own particular history and final structure might look like. My particular interest is in studying the unusual, often rapidly fading supernovae that may arise from massive stars that have undergone violent episodes near the end of their lives.

How have you benefitted from the SSGF Program?

The SSGF program has allowed me to focus on my research without worrying about the source of my funding, giving me the flexibility to try projects and choose my own research path without being constrained by advisors' needs or relying on Teaching Assistant positions. As I had only experienced research within the framework of academia, it has also been a valuable opportunity to work at a national laboratory during graduate school and gain a window into what a career at one of them might be like.

Have you spent time at one of the national laboratories?

I spent my practicum at Lawrence Livermore National Laboratory (LLNL) working with Laura Berzak Hopkins, a former fellow of the SSGF program, on inertial confinement fusion simulations. My graduate career has been very focused on the topic of supernovae, so it was extremely valuable to have an excursion into national laboratory applications of the same physics I have learned in the context of stellar explosions. It also invited me to start considering research careers outside the traditional academic route, which can offer equally stimulating work but at a different pace and with a different structure. Finally, my practicum and the SSGF annual meetings have allowed me to build a network of scientists outside the university system who are potential future collaborators and mentors.

Collin Stillman, University of Rochester (csti@lle.rochester.edu)

Degree in Progress: PhD, Physics ❖ University Advisors: Professors Philip Nilson and Dustin Froula ❖ SSGF Program: 2014-Present

Research Topic

Radiative properties at high energy density

What are your research responsibilities?

High-intensity, short-pulse lasers can be used to heat solid targets to temperatures above 1×10^6 K before hydrodynamic motion can occur, producing dense, high-temperature plasmas similar to those found in inertial confinement fusion (ICF) implosions and stellar interiors. Significant uncertainties exist in the radiative and material properties of matter within these systems due to the difficulty of obtaining homogeneous and well-characterized samples. My research focuses on understanding how to produce and characterize short-pulse laser plasmas for radiative properties studies. The experiments also provide a unique way to study plasma-dependent atomic properties in dense plasmas. I designed and built picosecond time-resolved x-ray spectrometers for these studies to record radiation emerging from the plasma. The spectra are used to understand the radiative properties of hot plasmas and provide data to test atomic physics models in high energy density systems.

How have you benefitted from the SSGF Program?

The SSGF program provides great opportunities for participants to interact with leading scientists in many different fields who are involved in cross-cutting and multidisciplinary research. These interactions consistently demonstrate the value of maintaining a broad appreciation of problem-solving techniques in diverse fields while gaining as much depth as possible in a focused area of study. In addition, the annual program review provides one of the best opportunities to learn from peers and connect with scientists at the NNSA national laboratories. These connections have helped provide a broader context for my own research and have uncovered future career opportunities in high energy density physics.

Have you spent time at one of the national laboratories?

I chose Lawrence Livermore National Laboratory for my SSGF practicum. I was able to spend three months onsite learning how to improve radiation-hydrodynamics modeling of short-pulse laser experiments from an expert. I gained substantial physical intuition by implementing simple ideas and observing how the model responded. This was especially valuable in a field where experimental time can be limited and experiments are difficult to diagnose. I learned how to think and approach problems as a theorist and saw how to apply the methods of computational experiment design. I also learned when and where model predictions are most reliable. The experience was an extraordinary opportunity to broaden my technical skill set and to learn physics beyond my immediate research interests.

Fabio Sanches, University of California, Berkeley (fabios@berkeley.edu)

Degree in Progress: PhD, Physics ❖ University Advisor: Professor Yasunori Nomura ❖ SSGF Program: 2013-Present

Research Topic

Theoretical high energy physics

What are your research responsibilities?

At high energies, our current description of particles and interactions no longer successfully explains how nature behaves. One of the most significant gaps in our understanding is at scales where the gravitational interaction is of equal or greater importance than the other forces. My research is focused on filling these gaps.

Currently, our most concrete description of gravitational phenomena comes from a framework called ‘holographic duality’. One example of this duality gives us an explicit relation between gravitational physics and certain theories that describe the fundamental particles and forces. Intuitively, a description similar to the one used for the strong interactions can be used to understand gravity, or vice-versa. Many of my recent projects have been aimed at expanding our understanding of this duality, and applying it in a broader setting. This means distilling which features are responsible for making the theories work and using them in a more general framework, as well as developing consistency checks.

How have you benefitted from the SSGF Program?

The SSGF program has really been important in my graduate career. As a starting point, their generous tuition and allowance support allowed me to focus on research from very early on. In addition, it provides a significant amount of academic freedom to explore problems and research ideas. The annual program review has also been a highlight of the program. I always look forward to learning about the breadth of research that other fellows and alumni are doing at universities and national laboratories. Furthermore, the SSGF allows us to explore the research being done at the national labs through the practicum and by interacting directly with top scientists during the meetings.

What do you want students considering the SSGF to know?

I am extremely grateful for the support and opportunities that the SSGF has provided. I would strongly encourage any student considering the SSGF to apply. The program will undoubtedly positively affect your career. In addition to the direct support, it provides a great community and mentorship that guides you towards excellent career possibilities after your PhD. Furthermore, it can help put you in contact with top researchers in many different fields, with positive influences on your work, and may even help you develop new research ideas!

Feature Articles

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Searching for Habitable Planets and Sustaining Our Nuclear Deterrent

Lawrence Livermore National Laboratory ❖ Author: Richard G. Kraus (kraus4@llnl.gov)

Figure 1. The artist’s concept depicts Kepler-186f, the first validated Earth-size planet to orbit a distant star in the habitable zone. Credits: NASA Ames/SETI Institute/JPL-Caltech.

We are searching for habitable exoplanets. The discovery of thousands of extrasolar planets, some close to Earth, some of similar size and surface temperature such as depicted in Figure 1, has captivated the public’s attention. The planetary science and astronomy communities state in their decadal research plans that finding habitable exoplanets is one of their top three goals; and the geophysics community works to understand how important processes like convection within the mantle and cores might differ in the large rocky extrasolar planets. However, there is a major gap in our understanding of these large rocky planets, dubbed *super-Earths*; the interior pressures are so extreme, up to 35 million times atmospheric pressure (35 Mbar), that we have very little information about how materials might behave within them. Do rocks become so strong that they cannot convect and help stabilize important geochemical cycles? Is the melting curve of iron so shallow that an inner core cannot solidify, limiting the chance for a geodynamo and therefore a protective magnetosphere? Answers to such questions determine the potential habitability of a planet.

One of the missions of the NNSA national laboratories is to ensure that the nation’s nuclear weapons stockpile is safe, secure, and reliable. To continue to achieve this mission requires a broad array of scientific expertise with validated experimental techniques and a continuous pipeline of excited scientists. One focus area common to all three NNSA laboratories is the response of materials to extreme conditions, in particular high pressures and temperatures. By participating in high-pressure planetology, the NNSA laboratories obtain a forum for vetting their experimental techniques and engaging students and postdoctoral researchers.

At Lawrence Livermore National Laboratory, we have begun a multi-institution collaboration to experimentally study the cores of exoplanets, with experts from George Washington University, the Carnegie DOE Alliance Center, the University of California Davis, the University College London, and the California Institute of Technology. Through the National Ignition Facility (NIF) Discovery Science program, we are attempting to measure the melt curve of iron at the extreme conditions found within super-Earths. As mentioned previously, the melting curve of iron is critical to our understanding of super-Earths habitability. For labs, melting curves represent the largest rheological transition a material can undergo, from a material with strength to one without; which is essential for simulating how a material flows under extreme dynamic loading.

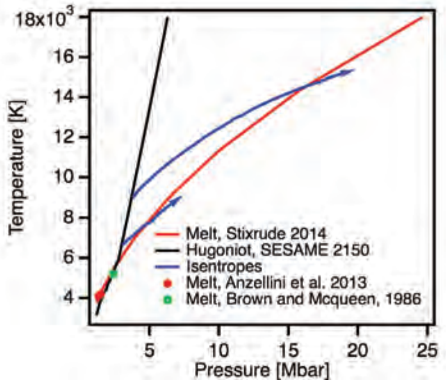

Figure 2. Phase diagram of iron over the pressure and temperature range of interest along with the current highest pressure data on the iron melt curve (red circles and green squares). The NIF experiments are designed such that the iron samples are shocked to a state on the Hugoniot[3] (black line) and then subsequently compressed along an isentropic path (blue lines) until the iron isentrope intersects the predicted melt curve[4] (red line) and the samples re-solidify at conditions comparable to those within super-Earths.

To reach the material states of interest (see Figure 2), we utilize the pulse shaping capability at the NIF. Sixteen beams directly ablate beryllium, driving a steady shock into the beryllium that transmits into our iron sample. This shock compresses and heats the iron until it reaches a liquid state. A few nanoseconds later, we increase the laser intensity and send a shockless compression wave into the liquid iron. Since shockless compression of a fluid lacks the dissipative effects of a shock, the compression is isentropic and the temperature remains relatively low. Once the iron reaches the desired compression, we fire more laser beams to rapidly heat a metallic foil to an x-ray emitting state. The emitted x-rays are collimated and diffracted by the iron sample, and collected using our x-ray diffraction diagnostic TARDIS (TARget Diffraction In Situ), shown in Figure 3. Within the collected x-ray signal, we look for diffraction lines, which indicate both the presence of solid iron and information about the crystal structure of the re-solidified iron. One

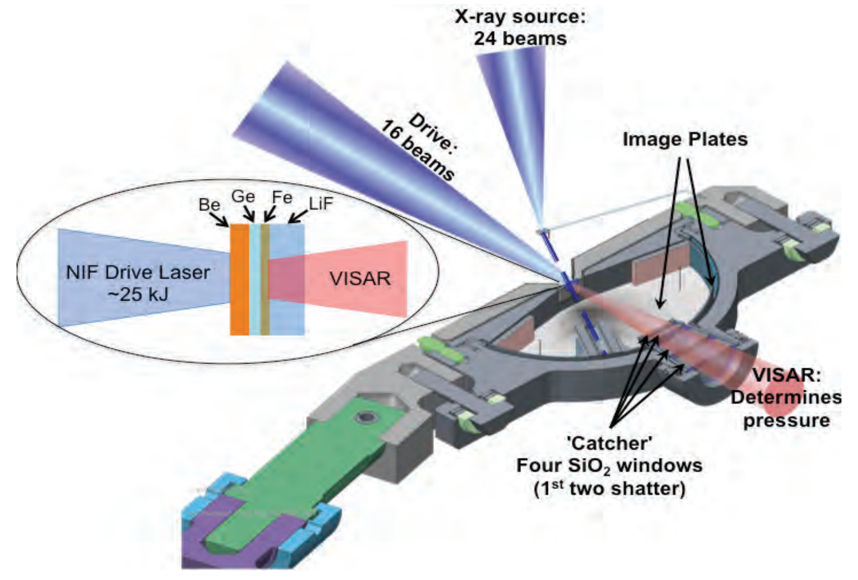

Figure 3. Schematic of the experiment. The TARDIS holds three image plates that collect the x-ray diffraction signal. The physics package is composed of a beryllium ablator, a germanium pre-heat shield, the iron sample, and a lithium fluoride window. The velocity interferometer system for any reflector (VISAR) measures the interface velocity between the iron and lithium fluoride to determine the pressure in the iron. The 'catcher' ensures that sample fragments are not shot out into the NIF chamber.

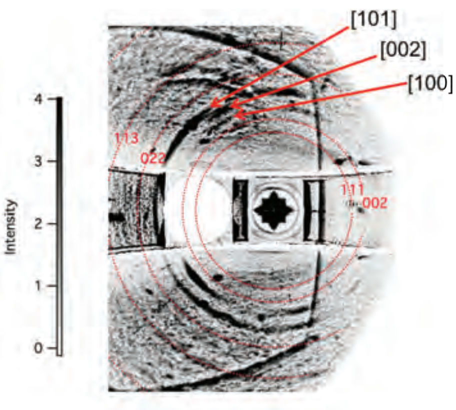

Figure 4. Stereographic projection in-situ x-ray diffraction from iron shocked to 2.3 Mbar then shocklessly compressed to 5.6 Mbar. Dotted red lines overlay the positions at which we expect diffraction from the platinum pinhole used to collimate the x-rays (Miller indices marked in red). Between the [002] and [022] platinum lines we observe three diffraction lines from the iron sample, indexed as the [100], [002], and [101] lines from the hexagonal close packed structure.

way to think about this experiment is that the shockwave creates a warm dense thermal state in the iron similar to that within the liquid iron outer core of a super-Earth. The subsequent shockless compression simulates the thermodynamic path experienced by a parcel of iron convecting deep within the liquid core of a super-Earth. We can directly answer the question of whether that parcel of iron would solidify as it reaches a prescribed depth.

We have been awarded experimental time at the NIF and by the time this publication comes out, we will have made significantly more progress. At this point, we have performed two developmental experiments, testing our hydrodynamic design and validating our capability to detect the signature of solid iron at such extreme conditions. In our most recent (August) experiment, we shock the compressed iron sample to 2.3 Mbar and then shocklessly increased the pressure in the iron sample to nearly 5.6 Mbar, or 1.5 times the pressure at the center of the Earth. In Figure 4, we present a stereographic projection of the scattered x-rays, showing the characteristic rings associated with diffraction from a crystalline solid. We observe three diffraction lines from the iron sample that we have indexed as originating from the hexagonal close packed crystal structure. While mainly a developmental test, this is also an important measurement as it is the only measurement of the phase of iron at such extreme conditions near the melt curve; it confirms that iron does not yet transform to any other phase such as the predicted body centered cubic structure.

We will continue to probe the crystal structure and melt curve of iron at conditions comparable to those within large terrestrial planets, from 5 to 20 Mbar. We will address the important question as to whether super-Earths could generate a protective magnetosphere, creating a stable and potentially habitable surface environment. And as we continue our discovery science, we are furthering our capability to explore important phenomenon in materials of interest to the NNSA.

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Calculating the Properties of Materials Using the World's Largest Computers

Sandia National Laboratories ❖ Author: Luke Shulenburger (lshulen@sandia.gov)

Electronic structure calculations inform vast swaths of work important to the mission of the NNSA national laboratories as well as much university research. From developing equations of state for hydrocodes to predicting the performance of electronics in a high radiation environment, the ability to calculate the properties of a material directly from first principles without empiricism is key to predictive science and reliable engineering. The current workhorse for these efforts is Density Functional Theory (DFT). Sandia National Laboratories (SNL) has decades of experience developing and applying this method including writing and maintaining two codes[1,2] and the development of new and improved approximations.[3] There are, however, several important classes of problems that have proven consistently difficult to treat with DFT. These include strongly correlated materials such as transition metal oxides, and materials where dispersion forces are important such as layered materials and molecular crystals.

Both cases are ideally suited to so-called many-body techniques. Rather than solving for independent particles in an effective potential as DFT traditionally does, many-body techniques directly confront the full complexity of the quantum mechanics of the interacting electrons. This sounds computationally expensive, and it is. For decades, however, computational capabilities have been growing at an astounding rate. The national laboratories have been at the forefront of this growth and for this reason are ideally suited to harness the power of the massively parallel computers of the future to make many-body physics calculations possible and perhaps one day routine. However, the task of developing methods and the infrastructure to make them useful is much too large for any single institution, and collaborations have proven crucial in this endeavor.

Given an algorithm suited to today's largest supercomputers, the appeal of many-body techniques becomes clear. Lacking an approximate Hamiltonian, electron localization, dispersion and other strong correlations become natural consequences of the calculations rather than difficult interactions to approximate. Over the last half decade, researchers at SNL have taken a much closer interest in quantum Monte Carlo (QMC) as a candidate to investigate and fill this need. QMC has the attractive trait that it is almost trivial to parallelize to the largest supercomputers in existence. One simply generates as many independent Markov chains as processing elements, and the only parallel bottlenecks come from occasionally collecting properties from these independent calculations or performing a rudimentary load balancing. Using this strategy, diffusion Monte Carlo calculations have been shown to scale to over 1.5 million simultaneously running central processing unit cores on the largest supercomputer at Lawrence Livermore National Laboratory (LLNL), Sequoia, as shown in Figure 1.

Quantum Monte Carlo calculations can be run efficiently on the world's largest computers

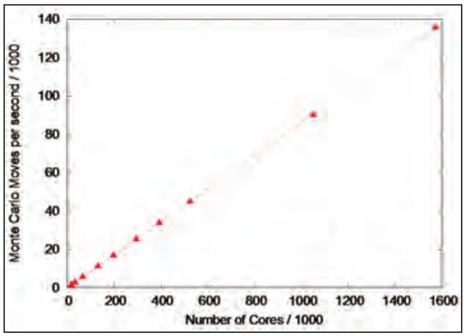

Figure 1. The rate of Monte Carlo moves grows linearly with processors on Sequoia, allowing over 1.5 million cores to be used simultaneously in a calculation of liquid xenon. This nearly ideal scaling enables much larger problems to be tackled than would otherwise be possible.

The code used for these calculations, qmcpack,[4] is a modern high performance C++ application that has been written from the ground up to take advantage of the architecture of the supercomputers of today and those expected to come in the future. This includes taking advantage of the difference between on-node and off-node communications and memory hierarchies, as well as leveraging the high performance of accelerators such as graphics processing units. SNL is jointly starting a multi-year program with researchers at Oak Ridge National Laboratory, Argonne National Laboratory, LLNL, Intel corporation, NVIDIA and Stone Ridge Technology to expand and deepen the current parallelization strategies in the code with an eye towards performance portability across the new architectures expected as computing moves into the Exascale era. In the short term, this collaboration will produce a series of publicly available mini-apps covering the computationally intensive parts of the code, with the goal of encouraging collaboration with computer scientists from other institutions to explore novel ways of parallelizing and optimizing these routines.

Benchmarks show quantum Monte Carlo is already among the most accurate methods available

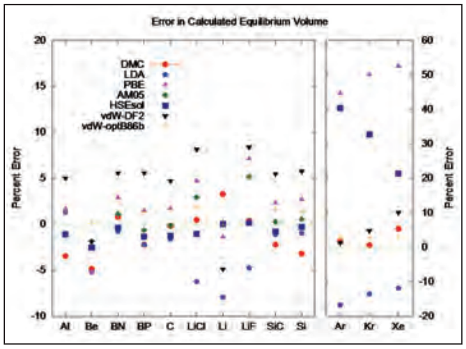

Figure 2. Compared to several of the most popular computational methods available, QMC demonstrates it is very accurate at predicting the equilibrium density of materials ranging from simple metals, to semiconductors, to noble gas solids. This plot shows the error in the calculated equilibrium volume of several materials with DMC (diffusion Monte Carlo) results shown in red and other symbols showing popular DFT approximations for comparison.

The computational aspect of the work is, however, only one part of the effort. The central question is how to take a theoretically appealing method and make it practically useful for the applications of interest. A hugely important aspect of this is understanding and reducing the approximations inherent in applying a method such as QMC. While benchmarks based on calculations of small molecules

Electron density is strongly affected by interlayer interactions in black phosphorus

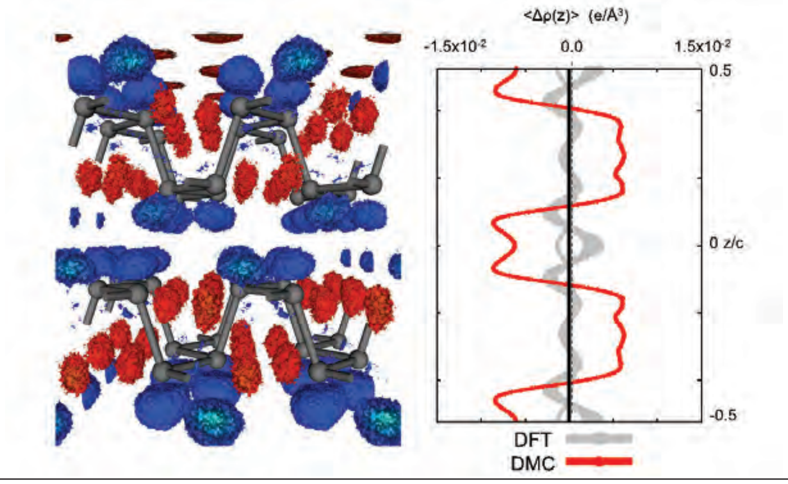

Figure 3. (Left) Charge reorganization induced by the interaction of black phosphorus layers. Phosphorus atoms and their bonds are shown in gray and areas where the electron density is reduced by the interlayer action are shown in blue, while regions where the electron density is increased are red. (Right) Large qualitative differences in charge transfer between DFT predictions (grey) and QMC (red). The change in charge density is integrated over the x-y plane and shown as a function of height in the material. Layers with reduced charge density fall to the left of the axis and with increased charge density to the right. This illustrates that the QMC calculation found a much stronger and qualitatively different charge redistribution than the DFT.

have been available for some time,[5] an understanding of the performance of these techniques for calculation of materials was lacking. In 2012, researchers at SNL took a step towards remedying this situation, publishing an extensive set of calculations of the properties of solids and comparing the results with both experiment and popular DFT approximations.[6] An example of these benchmark calculations is shown in Figure 2.

This work pointed to a previously unappreciated fact, that the effective interactions between core and valence electrons used for computational efficiency were having a larger impact on accuracy than the more fundamental approximations to the many-body physics. This observation spawned a collaboration between researchers at North Carolina State University and SNL to develop a new generation of these effective interactions that would come directly from knowledge of the many-body physics rather than being built on mean-field approximations. This work is currently ongoing, but this collaboration has already produced some of the most accurate potentials ever applied to many-body calculations and a methodology for constructing more as needed.

Despite the heavy focus on computational and algorithmic development, some of the most exciting aspects of the work have come from collaborating with academic researchers to apply QMC to new areas of physics and materials science. A recent example of this involved collaboration between the group of Professor David Tomanek at Michigan State University and SNL researchers Luke Shulenburger and Andrew Baczewski to understand the properties in black phosphorus. Black phosphorus is a layered material similar to graphite that can be exfoliated to produce nearly two dimensional sheets of the material that have great potential for application in electronics. Unlike the more widely studied graphene, single-layer black phosphorus, phosphorene, is inherently semiconducting, an ideal property for making devices. However, a key difficulty in making devices out of phosphorene is its tendency to degrade when exposed to air. Calculations to understand this require a knowledge of the way layers bind to themselves or to the substrates that they are attached to. Using quantum Monte Carlo, this collaboration showed that the binding between the black phosphorus layers was causing charge to rearrange in a way that had not been predicted, leading to a more complete understanding the physics necessary to stabilize single layers.[7] This charge reorganization is shown in Figure 3.

Despite the work that has already been done to bring QMC to the forefront of electronic structure, far more is yet to be accomplished. To this end, collaborations between researchers at the national laboratories and academic institutions will be essential to develop the method to its fullest potential.

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Ultrafast Visualization of Crystallization and Grain Growth in Shock-Compressed Condensed Matter

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The Shock and Detonation Physics Group at Los Alamos National Laboratory and Geological Sciences at Stanford University have recently taken advantage of the unique capabilities available at the Linac Coherent Light Source (LCLS), at SLAC National Accelerator Laboratory, to probe dynamic materials properties.

Understanding how matter transforms at the atomic scale is important for future design of material functionality. Pressure- and temperature-induced phase transitions have been studied for more than a century.[1,2] Little is known, however, about the non-equilibrium processes by which the atoms rearrange. Shock compression, the fastest mechanical loading that can be applied to a material, generates a nearly instantaneous propagating high-pressure/temperature condition, while *in situ* x-ray diffraction (XRD) probes the time-dependent atomic arrangement. Obtaining atomistic data in the non-equilibrium state during the process of a material phase transition has remained elusive until now. Combining shock-compression with the high-brightness short-pulse LCLS X-ray Free Electron Laser (XFEL) we report the first results of shock-induced nanosecond nucleation and growth of a high-pressure crystalline phase from initially amorphous material via ultrafast (i.e., femtosecond) diffraction.[3] We examine SiO_2, one of the most abundant materials in the Earth's crust, revealing its unexpectedly swift transformation to rare stishovite—a hard and dense mineral found naturally at impact sites on Earth's surface.[4]

A long-pulse optical laser incident on our SiO_2 sample generates plasma and the ablation process launches a shockwave. As this shock-front transits the sample, there is a change in the structural arrangement of the atoms. These structural changes are recorded as Debye-Scherrer patterns on downstream detectors. By varying the probe time of the x-rays with respect to the launching of the shockwave, we collect temporally-resolved XRD patterns clearly demonstrating the growth of crystalline stishovite out of the original amorphous fused silica (see Figure 1).

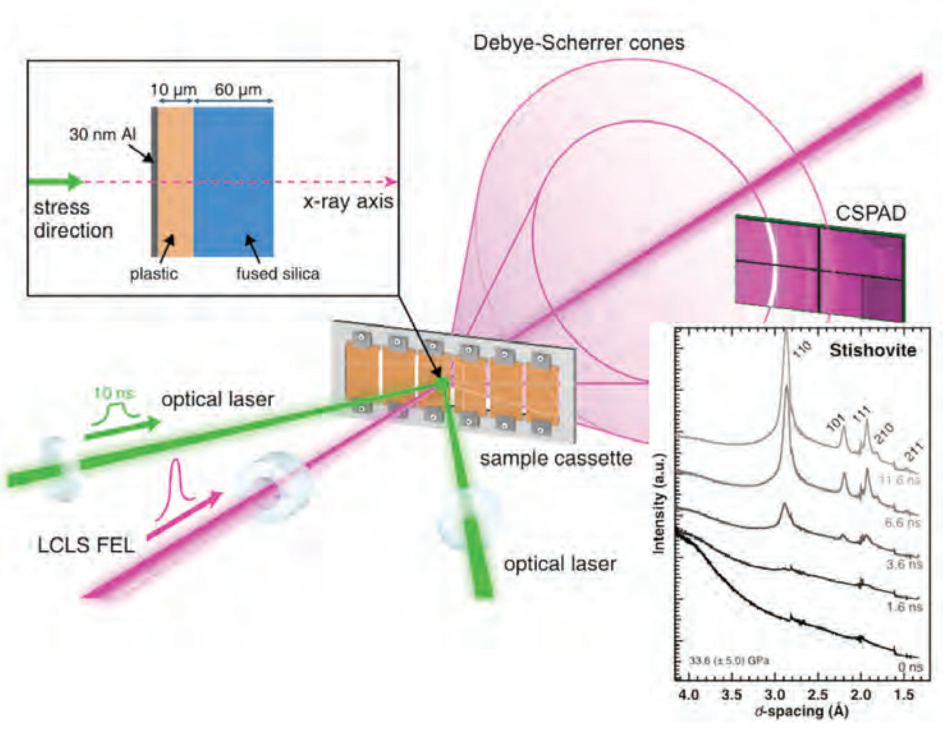

Figure 1. Experimental setup for visualizing grain nucleation and growth in a shock wave. The LCLS XFEL (pink) probes the sample at varying time-slices as the long-pulse laser (green) drives a shockwave to transit the sample. Detectors downstream (the Cornell-SLAC Pixel Array Detector, or CSPAD) capture the resultant Bragg peaks of the newly formed material with unparalleled spatial and temporal resolution.

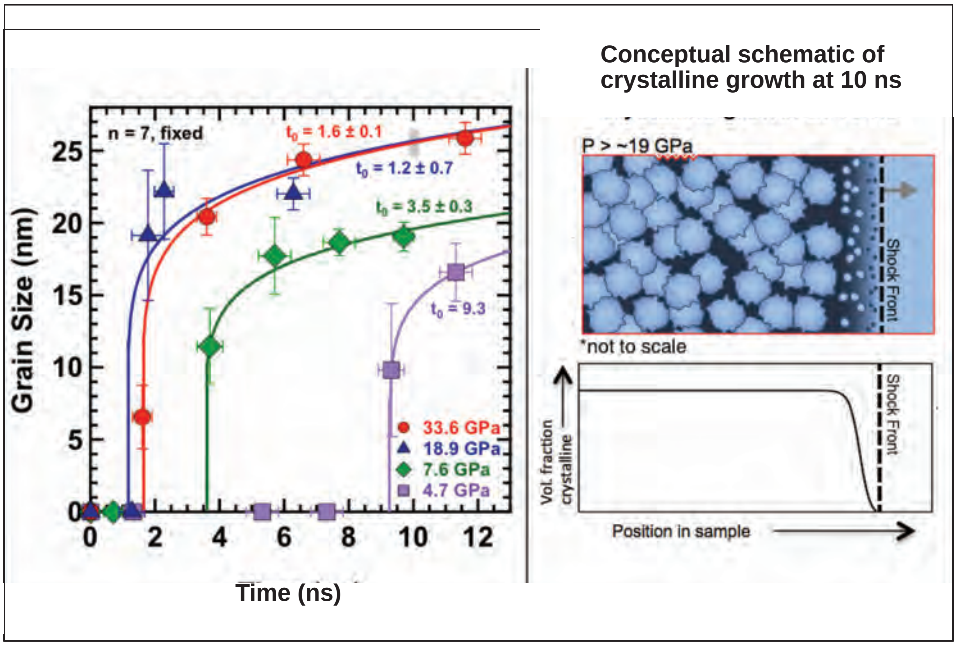

Figure 2. Conceptual schematic at pressures greater than 19 GPa of nano-crystalline stishovite grains coalescing rapidly and behind the shock front.

"These data and present analysis are the first demonstration of shock-induced crystallization of an amorphous material via femtosecond diffraction and are not only important to fundamental physics and geophysics, but will also lead to a greater understanding of phase transition kinetics and allow for advancements in material design and functionality. Our research supports the national security mission and materials modeling by showcasing a strategy and methodology to extract phase transition kinetics using time-resolved XRD data."

We measure the diffraction peaks widths which provide information on the size, and hence rate of growth of the nano-crystallites that form.[5] Though a disorder to ordering process is expected to be slow, we find that the stishovite grains nucleate and grow rapidly, within the first few nanoseconds, and the growth trend supports a coalescence growth model rather than a diffusion-based mechanism (see Figure 2).

These data and present analysis are the first demonstration of shock-induced crystallization of an amorphous material via femtosecond diffraction and are not only important to fundamental physics and geophysics, but will also lead to a greater understanding of phase transition kinetics and allow for advancements in material design and functionality. Our research supports the national security mission and materials modeling by showcasing a strategy and methodology to extract phase transition kinetics using time-resolved XRD data. Extensions of this work aim to allow structural determination of non-crystalline materials and by performing the time-dependent measurements on a single shock event for measurements of crystallization dynamics near phase boundaries.

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LDRD and SDRD: Training Grounds for the Next-Generation NNSA Workforce

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Among the greatest challenges facing the National Nuclear Security Administration's (NNSA's) Offices of Inertial Confinement Fusion, Science, and Advanced Scientific Computing are the development and integration of the next-generation workforce. The DOE/NNSA national laboratories, sites, and NNSA have developed partnerships with universities across the country to produce doctoral graduates with the skills needed for the science of nuclear security, and most new graduates enter the NNSA as postdoctoral researchers ("postdocs"). Integrating postdocs into the NNSA's core missions is a process because they require time to get up to speed on the science of the Defense Programs and Global Security missions. Bridging this gap, while also driving scientific and technical innovation, the Laboratory and Site-Directed Research and Development (LDRD/SDRD) programs provide projects where researchers new to the NNSA can make an immediate impact and gain important new skills for solving the future problems of the Nation.

Established in 1991, LDRD/SDRD is the national laboratories' and site's program for discretionary research, with projects derived bottom-up from the principal investigators (PIs). The projects are designed to support DOE's national security mission and are selected competitively to maintain each laboratories' and site's intellectual vitality, to respond immediately to developments at the cutting edge of science and technology, and to retain the best scientific, technical, and managerial talent (DOE Order 413.2B). To achieve these goals—and to serve as a training ground for new NNSA researchers—more than half of all postdocs at the NNSA laboratories and site are at least partially funded to work on LDRD projects.[1,2,3,4]

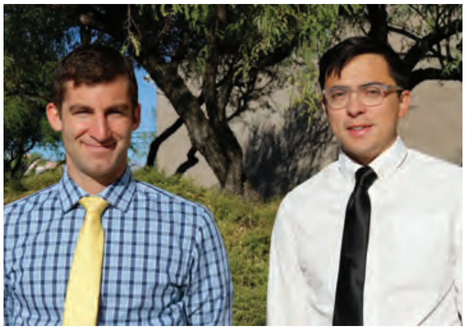

Figure 1. Jared Catenacci (left) and Kevin Joyce of NNSS.

At the Nevada National Security Site (NNSS), and in the Nevada Enterprise more broadly, SDRD projects are often used to fund graduate students before they even join the NNSS staff. Kevin Joyce began with the Diagnostic Research and Material Studies group in North Las Vegas (NLV) in 2013, when he was still a graduate student. His doctoral work, funded under an SDRD project titled "Quantifying Uncertainties Through Advanced Theoretical Analysis for Image and Signal Reconstruction," focused on developing new mathematical models for characterizing the impulse response of the Cygnus x-ray source at the NNSS. Joyce finished his PhD in Mathematics in May 2016 at the University of Montana, and he joined the NLV team as a postdoc in June 2016, where he is continuing his connection to SDRD. Joyce notes, "My PhD work came directly from questions posed on an SDRD project, so it is natural for me to continue in that arena as a postdoc." He is looking forward to using SDRD as a means to grow his technical expertise, by expanding to a second SDRD project with Global Security applications. According to Joyce, "My next SDRD project involves predicting dynamic experiments through fusing remotely sensed data using state of the art multi-source data fusion techniques." This is a project that is being led by another new postdoc, Jared Catenacci, who finished his PhD in Mathematics at North Carolina State University in 2016. Upon joining the NLV group in July, he immediately took the lead role on the SDRD project titled "Dynamic Test Prediction and Characterization Through Modeling-informed, Multi-Source Data Fusion." This has helped his transition to the NNSA by approaching questions of programmatic importance in a way to which a recent graduate student is accustomed. According to Catenacci, "In many ways, SDRD work is very academic; we're asking interesting questions and trying to come up with innovative methods for solving the problems. That being said, the questions we're trying to answer are directly motivated by problems encountered at the programmatic level. In this way, our SDRD work is providing a lens through which to see what the important and challenging issues are from a programmatic standpoint, while still being able to conduct research with an academic mindset." For both Joyce and Catenacci, SDRD has provided the basic research opportunities that balance their more applied programmatic work at the outset of their postdoctoral careers at the NNSS.

Figure 2. Brian Shaw (left) and Sheng Jiang of LLNL.

At Lawrence Livermore National Laboratory (LLNL), Brian Shaw and Sheng Jiang (see Figure 2) are in the middle of their postdoctoral research appointments in the Accelerators Group of the National Security Engineering Division, where they are developing new approaches to modeling fusion plasmas on an LDRD project titled "A Dense-Plasma Focus (DPF) Device as a Compact Neutron Source." Shaw completed his PhD in Applied Science and Technology at the University of California, Berkeley in 2015, and LDRD is giving him a broad introduction to LLNL's mission space. "This project

Figure 3. Kyle Hickman (left) and Kendra Van Buren of LANL.

Quick Facts

Postdoctoral Researchers Supported by LDRD

	Total # of Postdocs Supported by LDRD	Percentage of Lab/Site Postdocs Supported by LDRD
SNL[1]	278	51
LANL[2]	266	55
LLNL[3]	102	43
NNSS[4,*]	2	100

[*] Fixed term post-doctoral employment was incorporated into the NNSS Prime Contract in FY 2015.

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enhances capabilities in fully kinetic z-pinch modeling, a component of the Laboratory's high-energy-density science core competency. Our work also enables applications in the strategic focus area of stockpile stewardship science, in which the predictive capability for nuclear weapon performance requires fundamental understanding of extreme, high-energy density states of matter." Sheng Jiang, who received her PhD in Physics in 2015 at The Ohio State University, also works on the DPF project, which is a different direction in her research. "The physics of dense plasma focus devices is new to me, since I worked mostly on laser-plasma interactions as a graduate student. Nonetheless, a lot of the knowledge and metrologies are quite similar, so it has been a smooth transition to apply the skills that I learned before." This project has also allowed her to have a broader scientific impact than she previously had, with LLNL growing their DPF capabilities and taking an active role in the development of pulsed neutron sources for future hydrodynamic and subcritical nuclear experiments. Sheng adds, "In addition to trying to explain the experimental results, we modelers now also have a great contribution in planning and designing the experimental devices that will be used in new LLNL programs, really expanding the impact of our work."

In Fiscal Year (FY) 2016, Kyle Hickmann and Kendra Van Buren both converted from being postdocs to staff scientists in the Los Alamos National Laboratory (LANL) Computational Physics Validation and Analysis Group. Hickmann, who received his PhD in Mathematics from Oregon State University in 2010, was a research postdoc on a project titled "Reducing Data Dimensionality in Seismic Inversion," whose primary goal was to develop state-of-the-art machine learning tools to eliminate redundancies in large seismic data sets. His LDRD experience offered him exposure to other projects and people with whom he might not have otherwise interacted. He notes, "Through this project, I was introduced to many senior researchers working in more programmatic areas, and it led directly to my conversion to a staff position." Although only recently converted to staff, Van Buren is already an experienced LANL scientist, having begun working at LANL while still a graduate student at Clemson University, where she received her PhD in Civil Engineering in 2012. As a doctoral student, Van Buren worked on an LDRD project titled "Intelligent Wind Turbines" and, as a postdoc, she was the principal investigator (PI) on an LDRD program development project titled "Addressing the Multi-Intelligence Challenge through Robust Decision-Making," for which Van Buren received a LANL FY 2015 Postdoc Distinguished Performance Award. Her LDRD experience taught her more than just new science. "I worked on a large, multi-disciplinary team, which meant I was interacting with people who have vastly different backgrounds from mine. This required that I learn how to effectively communicate with other scientists and decision makers who think differently about the work than I do, which is an essential skill for success in the laboratory." Serving as an LDRD PI also gave Van Buren the opportunity to grow as a scientific leader. She adds, "My postdoctoral research was different than what I did during my PhD and really helped demonstrate to my group leader that I was capable of working on new projects and learning new things. It helped me grow scientifically, but also as a leader." For both Hickmann and Van Buren, LDRD provided the scientific transition to being successful now as staff scientists.

In FY 2015, there were over 600 postdoctoral researchers supported by LDRD at the NNSA laboratories and NNSS. Each laboratory takes a different approach to how LDRD is used to integrate new scientists into its research, but all have in common that LDRD allows postdocs the opportunity to train in the laboratories' missions, to transition from their experiences in academia to working in the laboratory or site environment, and to grow technically as scientists and future laboratory and site leaders.

Probing Materials Under Extreme Conditions Using Synchrotron Radiation

High Pressure Collaborative Access Team ❖ PIs: Drs. Guoyin Shen (gshen@ciw.edu) and Russell J. Hemley (rhemley@gwu.edu)

Pressure profoundly alters matter and materials. The development of ultrahigh-pressure devices, to compress samples to sustained multimegabar pressures together with synchrotron x-ray techniques to probe material properties *in situ*, has enabled the exploration of novel properties of materials at extreme conditions. The NNSA-sponsored High Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source (APS), Argonne National Laboratory (ANL) is a frontier synchrotron facility optimized for high-pressure studies designed to advance our understanding of materials of importance for Stewardship Science (see Figure 1). These studies include the following:

- *x-ray emission spectroscopy*, which provides information on the filled electronic states of samples;
- *x-ray Raman spectroscopy*, which probes the chemical bonding changes of light elements;
- *electronic inelastic x-ray scattering spectroscopy*, which accesses high energy electronic phenomena, including electronic band structure, Fermi surface, excitons, plasmons, and their dispersions;
- *nuclear resonant x-ray spectroscopy*, which provides phonon densities of state and time-resolved Mössbauer information;
- *x-ray diffraction*, which determines the fundamental structures and densities of single-crystal, polycrystalline, nanocrystalline, and non-crystalline materials; and
- *radial x-ray diffraction*, which yields deviatoric, elastic and rheological information.

Integrating these tools with hydrostatic or uniaxial pressure media, rapid compression and decompression, pulsed and modulated laser heating, and resistive heating and cryogenic cooling, has enabled investigations of the structural, vibrational, electronic, and magnetic properties of materials over a wide range of pressure-temperature conditions, isothermal (de)compression rates, and isobaric heating/cooling rates. Figure 2 shows an example of the capabilities of x-ray emission spectroscopy during compression.

More than 25,000 hours per year of synchrotron beamtime are delivered for exploring matter under extreme conditions using the dedicated facility. More than 250 individual users per year come to HPCAT performing high-pressure synchrotron experiments. If counting the returned users, the number of person-visits is greater than 550 per year. In addition to numerous reports to the NNSA programs, research activities at HPCAT result in more than

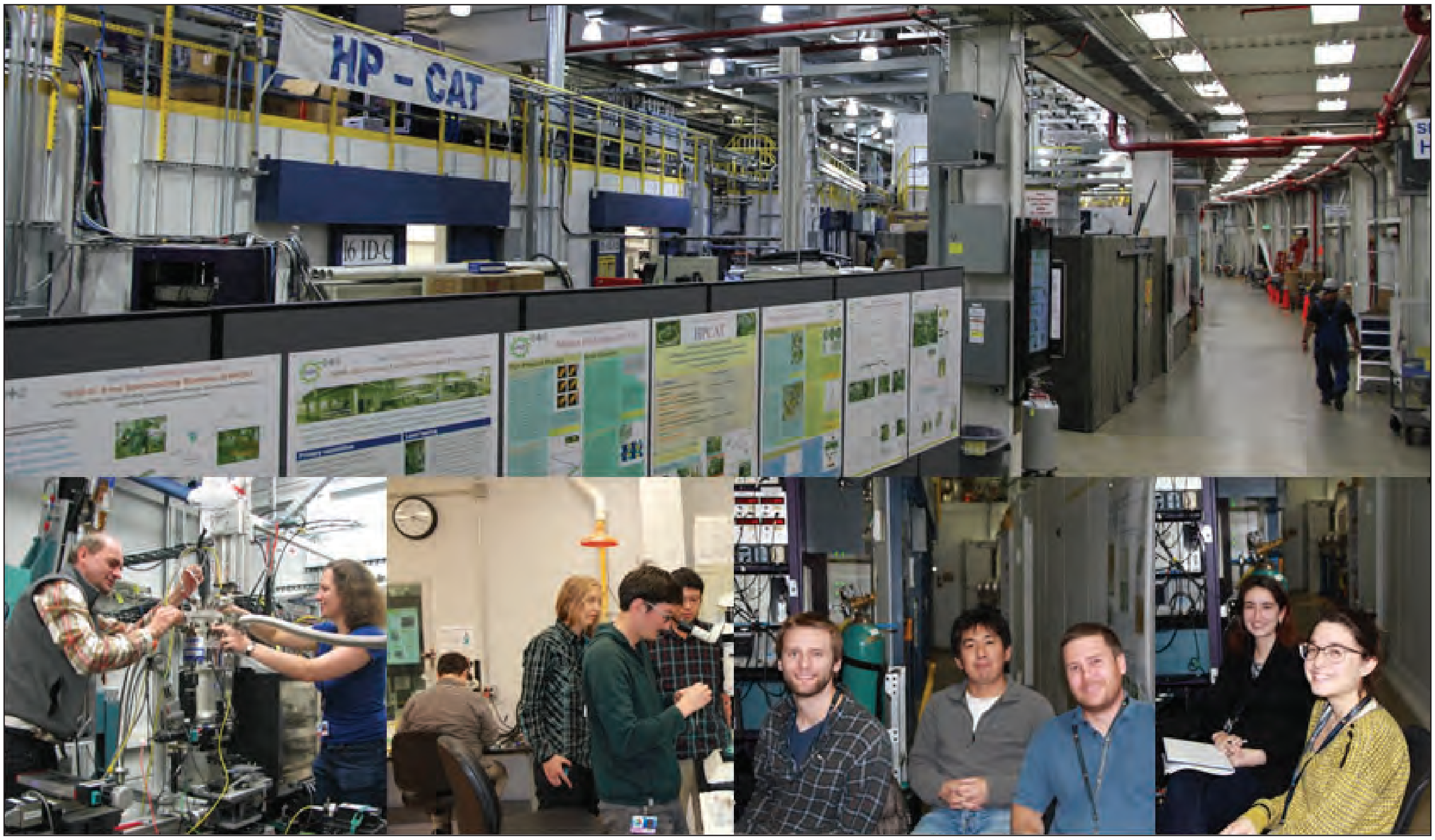


Figure 1. HPCAT at the APS. At HPCAT, 62% of the users are graduate students or postdoctoral scientists, making the facility an important training ground for next-generation scientists with the state-of-the-art equipment for materials studies.

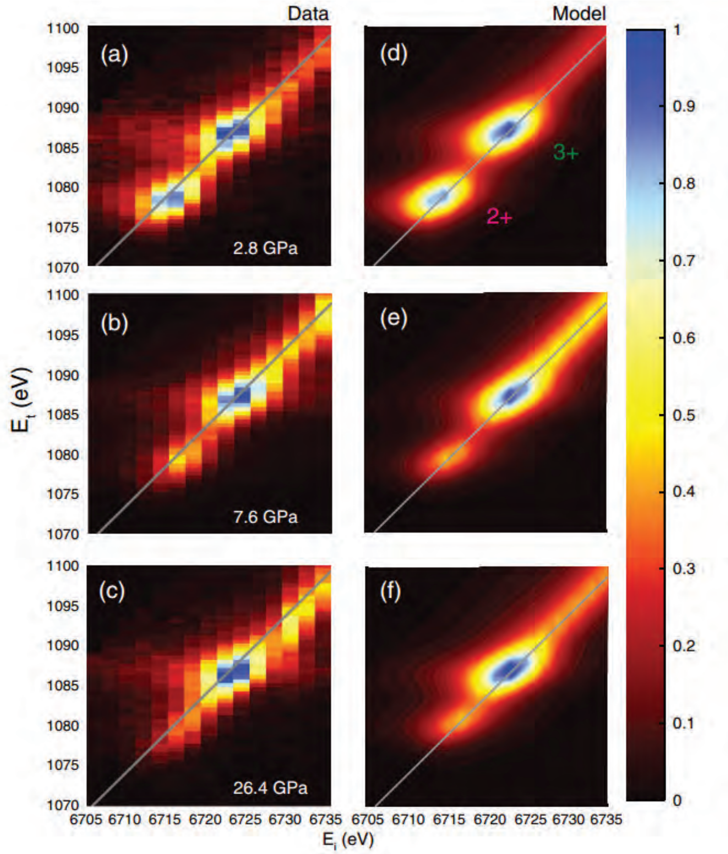


Figure 2. The pressure dependence of the f-electron occupancy in Kondo insulator SmB$_6$, revealed by resonant x-ray emission spectroscopy (RXES) in which both incident energy E_i and transferred energy E_t=E_i-E_f are varied, here E_f is the emitted energy. (a-c) Experimental RXES data; (d-f) the theoretical fits. The gray lines denote constant values of E_f corresponding to the fluorescence line. [Phys. Rev. Lett., 116, 156401, 2016]

> *"More than 250 individual users per year come to HPCAT performing high-pressure synchrotron experiments. If counting the returned users, the number of person-visits is greater than 550 per year. In addition to numerous reports to the NNSA programs, research activities at HPCAT result in more than 110 peer-reviewed papers per year in the past three years. Every year, more than 10 PhD theses and 3 Masters theses are completed based at least in part on experiments performed at HPCAT."*

* * *

110 peer-reviewed papers per year in the past three years. Every year, more than 10 PhD theses and 3 Masters theses are completed based at least in part on experiments performed at HPCAT.

In the past year, several new techniques and capabilities have been established at HPCAT. They include the following:

- *Time resolved x-ray diffraction* at micro-second level with the laser heating system has been successfully commissioned.
- *On-the-fly sample mapping* with integrated x-ray diffraction, coupled with the newly established beam-size of 1×2 μm^2, opens the studies of complex and heterogeneous samples and combinatorial experiments.
- A new method for *high pressure melting* has been established for metals, with melting curves for Mo and Fe determined to over 2 megabars.
- A new *two-stage assembly* has reached a pressure of >130 GPa in a Paris-Edinburgh press, enabling structural studies of weak scattering materials (e.g., liquid and amorphous) to megabar pressures.

In the light of the APS Upgrade and novel synchrotron techniques that have become feasible and practical, HPCAT is entering a new era in compression science. The APS Upgrade will provide a 100 to 1,000 times increase in brightness and coherence at high energy that will dramatically improve the ability to study smaller samples with finer temporal resolution and greater precision and accuracy. New developments in synchrotron techniques, together with advanced detectors and high power computing algorithms, provide unprecedented opportunities for probing matter under extreme conditions, such as redefining the scope of research by extending pressures beyond 0.5 TPa; revolutionary understanding of complex materials across the entire hierarchy of length scales and heterogeneity of materials at high pressure; studying kinetics, pathways, and metastability under rapid (de)compression and pulsed (or modulated) laser heating at high pressure; accurately probing phase transitions and chemical reactions at megabar pressures; high throughput characterization probes for exploiting extreme environments for materials design, pathways, and synthesis.

List of Grants and Cooperative Agreements

Stewardship Science Academic Alliances

High Energy Density Physics

Cornell University
Bruce Kusse and David Hammer
Center for Pulsed-Power-Driven High Energy Density Plasmas

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

University of Michigan
Karl Krushelnick
Relativistic Laser Plasma Interaction at the University of Michigan

University of Nevada, Reno
Aaron Covington
Investigations of High Energy Density Plasmas at the Nevada Terawatt Facility and Beyond

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

Oregan 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
Neutron-Induced Fission in the Actinides: Neutron Energy-Angle Correlations, and Extended-Energy Yields

University of Kentucky
Steven Yates
Elastic and Inelastic Neutron Scattering Differential Cross Sections on Iron, Silicon, and Carbon

University of Massachusetts Lowell
Partha Chowdhury
Nuclear Science with a C7LYC Array (SCANS)

University of Richmond
Con Beausang
Stewardship Science at the University of Richmond

University of Tennessee
Robert Gryzwacz
New High Resolution Neutron Detector for the Studies of Exotic Nuclei (NEXT)

Properties of Materials Under Extreme Conditions

Arizona State University
Pedro Peralta
Formulation and Validation of Anisotropic Models for Growth and Coalescence of Spall Damage in Crystalline Materials

Carnegie Institution of Washington
Stephen Gramsch
Carnegie/DOE Alliance Center: A Center of Excellence for High Pressure Science and Technology

Carnegie Mellon University
Robert Suter
Towards Optimal Processing of Additive Manufactured Metals for High Strain Rate Properties

Case Western Reserve University
Vikas Prakash
Dynamic Shearing Resistance of Metals Under Extreme Conditions

Georgia Tech
Devesh Ranjan
Detailed Measurements of Turbulent Rayleigh-Taylor Mixing at Large Atwood Numbers

Harvard University
Isaac Silvera
High Pressure Metallic Hydrogen

Lehigh University
Arindam Banerjee
The Effects of Materials Strength and De-Mixing on Rayleigh Taylor Turbulence

Stanford University
Mark Cappelli
Ultra-High Speed Neutral Plasma Jets and Their Interactions with Materials Generating Extreme Conditions

Stony Brook University
Baosheng Li
Thermodynamic and Mechanical Properties of SSP Materials from Simultaneous Ultrasonic and X-ray Studies at High Pressure and Temperature

Texas Tech University
Hongxing Jiang
Fast Neutron Spectrometry, Dosimetry, and Directionality Monitoring Using Semiconductor Thin Film Detector Arrays

University of Alabama at Birmingham
Yogesh Vohra
Studies on Rare Earth Metals and Alloys Under Extreme Conditions in Support of the Stockpile Stewardship Program

University of Arizona
Jeffrey Jacobs
An Experimental Study of the Turbulent Development of Rayleigh-Taylor and Richtmyer-Meshkov Instabilities

University of California, Davis
Richard Scalettar
Spectroscopic and Nuclear Magnetic Resonance Studies of Screening in Compressed Novel Magnets: Rare Earth and Fe-based Compounds

University of California, Santa Barbara
Tresa Pollock
New Multimodal Characterization of Additive Structures for Extreme Environments

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

University of California, San Diego
Marc Meyers
Viscous Plastic Flow, Dislocation Velocities, and Amorphization at Extreme Pressures and Strain-Rates

University of Illinois at Urbana-Champaign
David Ceperley
Quantum Simulations for Dense Matter

University of Missouri
Jacob McFarland
Richtmyer-Meshkov Instability of a Plasma Cylinder with Magnetic Effects

University of Nevada, Las Vegas
Andrew Cornelius
High Pressure Science and Engineering Center

University of Nevada, Las Vegas
Michael Pravica
Development of Useful Hard X-ray Induced Chemistry

University of New Mexico
Peter Vorobieff
Quantification of Normal and Oblique Shock-Driven Phase Interaction and Transition to Turbulence in Media with Multiscale Density Interfaces

University of Wisconsin, Madison
Riccardo Bonazza
Investigation of the Turbulent Mixing in a Twice-Shocked Interface

University of Wisconsin, Madison
Zhenqiang Ma
Membrane Enabled Hard X-ray Imager (MEHXI)

Washington State University
Yogendra Gupta
Institute for Shock Physics

Washington State University
C.S. Yoo
Planetary Materials under Extreme Conditions

Wichita State University
Viswanathan Madhavan
Extreme Condition Mechanical Testing of AM Materials Using Complementary Methods

Radiochemistry

Clemson University
Timothy DeVol
Robust Extractive Scintillating Resin and Adsorptive Membranes for Plutonium Isotopic Analyses of Aqueous Media

University of Tennessee
Howard Hall
University of Tennessee Radiochemistry Center of Excellence

Washington State University
Nathalie Wall
Determination of Thermodynamic and Kinetic Parameters for Complexation of Tc(IV) with F-, Cl-, Br-, I-, SO42- and PO43-, acetate, citrate and EDTA

Other

California Institute of Technology
Paul Dimotakis
A New Computational Fluid Dynamics Framework for Multi-Physics Simulations

Carnegie Institution of Washington
Guoyin Shen
High Pressure Collaborative Access Team (HPCAT) Operations

Washington State University
Yogendra Gupta
Dynamic Compression Sector (DCS) Development at the Advanced Photon Source

High Energy Density Laboratory Plasmas

Cornell University
John Greenly
Magnetized High Energy Density Plasma Flows Drive By Skin Effects

Harvard University
Stein Jacobsen
From Z to Planets: Phase II

Massachusetts Institute of Technology
Richard Petrasso
Studying Hydrodynamics, Kinetic/multi-ion Effects, and Charged-Particle Stopping in HED Plasmas and ICF Implosions at OMEGA, OMEGA-EP, and at the NIF

Polymath Research, Inc.
Bedros Afeyan
Continuation of Statistical Nonlinear Optics of High Energy Density Plasmas: The Physics of Multiple Crossing Laser Beams

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

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

University of California, Los Angeles
Warren Mori
Continuation of the Application of Parallel Kinetic Simulations to Laser and Electron Transport Through High Energy Density Laboratory Plasmas

University of California, Los Angeles
Chand Joshi
Development of a Broadband (40-80 KV), Directional X-ray Source Platform for Radiography of HEDP Targets

University of Michigan
R. Paul Drake
Center for Laser Experimental Astrophysics Research

University of Nevada, Reno
Alla Safronova
Line Emission from High-Z Multiple Ionized Ions Influenced by Dielectronic Recombination and Polarization

National Laser Users' Facility

General Atomics
Mingsheng Wei
Hot Electron Scaling in Long Pulse Laser Plasma Interaction Relevant to Shock Ignition

Massachusetts Institute of Technology
Richard Petrasso
Explorations of Inertial-Confinement Fusion, High-Energy-Density Physics, and Laboratory Astrophysics

Princeton University
Amitava Bhattacharjee
Dynamics of Magnetic Reconnection and Instabilities of Current Sheets in High-Energy-Density Plasmas

Princeton University
Thomas Duffy
Dynamic Compression of Earth and Planetary Materials Using the Omega Laser

Princeton University
Anatoly Spitkovsky
Generation of Collisionless Shocks in Laser-Produced Plasmas

University of California, Berkeley
Raymond Jeanloz
Exploring the Quantum Mechanics of Dense Matter

University of California, San Diego
Farhat Beg
Fast Electron Energy Coupling and Transport in Warm Dense Plasmas

University of Chicago
Don Q. Lamb
Non-Linear Amplification of Magnetic Fields in Laser-Produced Plasmas

University of Michigan
R. Paul Drake
Experimental Astrophysics on the Omega Laser

University of Michigan
Louise Willingale
High-energy Electron Beam Acceleration from Underdense Plasma Using OMEGA-EP

University of Michigan
Karl Krushelnick
X-ray Measurements of Laser-Driven Relativistic Magnetic Reconnection Using OMEGA-EP

William Marsh Rice University
E.P. Liang
Creation of Magnetized Jet Using a Hollow Ring of Laser Beams

William Marsh Rice University
Patrick Hartigan
Astrophysical Dynamics in the Laboratory: Mach Stems and Magnetized Shocks

Predictive Science Academic Alliance Program II

Stanford University
Gianluca Iaccarino
Predictive Simulations of Particle-Laden Turbulence in a Radiation Environment

Texas A&M University
Jim Morel
Center for Exascale Radiation Transport

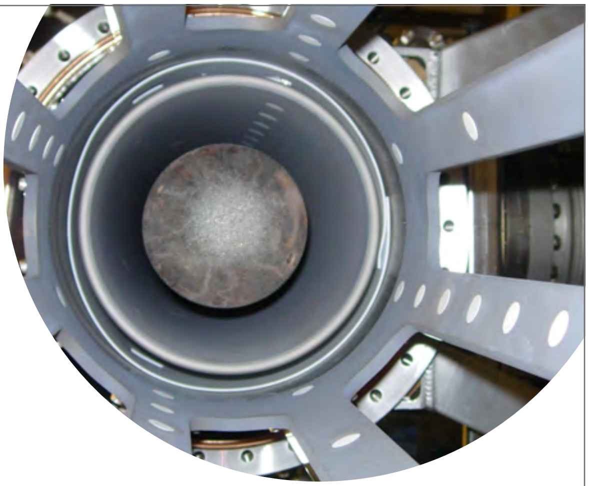
The University of Utah
Philip J. Smith
Carbon Capture Multidisciplinary Simulation Center

University of Florida, Gainesville
S. Balachandar
Center for Compressible Multiphase Turbulence

University of Illinois at Urbana-Champaign
William Gropp
The Center for Exascale Simulation of Plasma-Coupled Combustion

University of Notre Dame
Karel Matous
Center for Shock Wave-Processing of Advanced Reactive Materials

https://www.nnsa.energy.gov/stockpile stewardship



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Department of Energy National Nuclear Security Administration

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The Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) program provides outstanding benefits and opportunities to students pursuing a Ph.D. in areas of interest to stewardship science, such as properties of materials under extreme conditions and hydrodynamics, nuclear science, or high energy density physics. The fellowship includes a 12-week research experience at Lawrence Livermore National Laboratory, Los Alamos National Laboratory or Sandia National Laboratories.

APPLY ONLINE | The DOE NNSA SSGF program is open to senior undergraduates or students in their first or second year of graduate study. Access application materials and additional information at:

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Renewable up to four years

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

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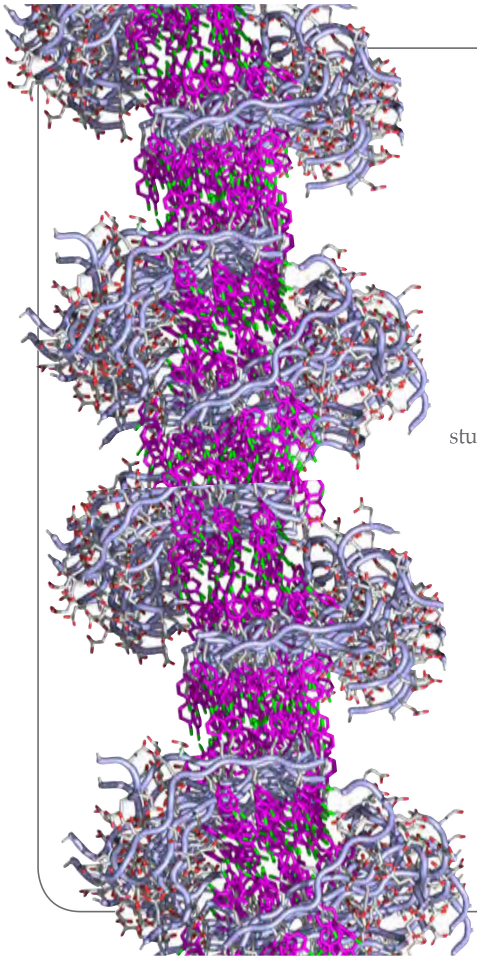

DOE CSGF

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COMPUTATIONAL SCIENCE GRADUATE FELLOWSHIP

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BENEFITS >

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$5,000 academic allowance in first year / 12-week research practicum
Renewable up to four years / $1,000 academic allowance each renewed year

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