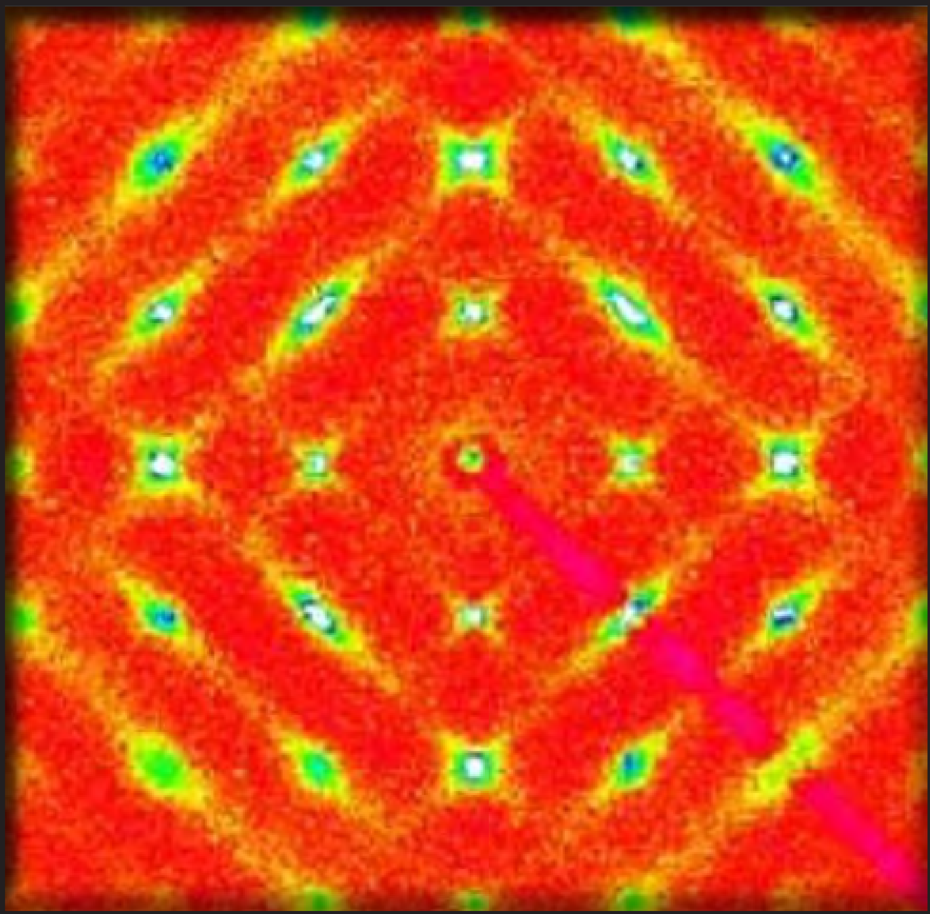
National Nuclear Security Administration

DOE/NA-0019

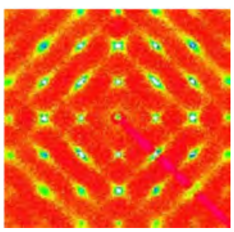
2013

# Stewardship Science Academic Programs Annual

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



U.S. DEPARTMENT OF ENERGY



## On the cover

A charge coupled device image of diffuse x-ray scattering from the ferroelectric material Pb(Sc,Nb)O3 taken at 16-ID-B at the High Pressure Collaborative Access Team by Muhtar Ahart, a research scientist at the Carnegie Institution of Washington.

— *Carnegie/DOE Alliance Center (CDAC)*

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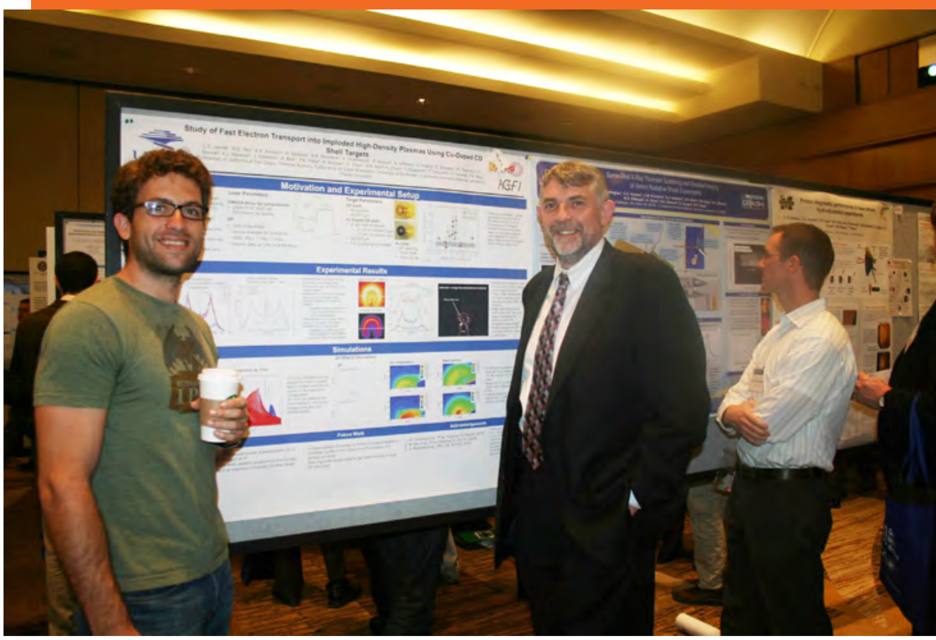


Dr. Christopher Deeney (middle) with attendees of the Poster Session during the 2012 Stewardship Science Academic Alliances Symposium. Last year's event, held at the Hyatt Regency in Washington, DC on February 22-23, 2012, hosted more than 275 attendees.

Mission First
Through Teamwork

## Message from the Assistant Deputy Administrator for Stockpile Stewardship

Each year, I look forward to this opportunity to communicate to you—the next generation of nuclear security stewards. This year, we are faced with many new challenges as well as an increasing need to be agile and responsive to a diverse set of important and exciting national security issues.

The primary mission of NNSA is to ensure a safe, secure and effective nuclear deterrent, and over the last two decades we have done so without nuclear testing. Today, we remain diligently focused on this mission and are grateful for the many former participants from the Stewardship Science Academic Programs (SSAP) that have chosen a career with the NNSA National Laboratories. They continue to be an important part of this success.

As we continue to make reductions to the nuclear force, it is important to remember that these are not reductions in nuclear deterrence, but rather reductions in the raw number of nuclear weapons populating the U.S. stockpile. The mission, therefore, for science-based stewardship has never been more important. The requirements for assessing the effectiveness of the nuclear deterrent without nuclear testing increase when decreasing the size of the stockpile. We will continue to make strong investments in science, and in the next generation of scientists and engineers for the national laboratories, despite extreme budget pressures we will face over the coming decade.

There are significant scientific and technological challenges with stewarding the nuclear deterrent, but we must never lose sight of the key role the laboratories play in our national security. As an example, let's consider what has happened in the world since last year's Annual was published:

- North Korea conducted a third nuclear test;
- Iran amassed new centrifuges for uranium enrichment; and
- the International Atomic Energy Agency announced that they believe Iran is conducting explosive tests for nuclear design.

In all three cases, NNSA is leading key efforts to assess their impacts and to inform top U.S. leadership. Our laboratories are asked to provide their expertise to a wide range of national security problems because the experimental and computational needs of the stockpile stewardship mission intersect the needs for these issues as well. The quality of these capabilities will only remain healthy by maintaining a strong laboratory workforce and a strong network of external subject matter experts for technical peer review

My door is always open to discuss career opportunities at the laboratories. Thank you for dedicating your intelligence and energy to the scientific disciplines within the SSAP.

Dr. Christopher Deeney
Assistant Deputy Administrator
for Stockpile Stewardship

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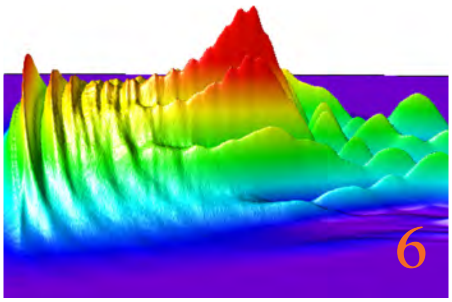


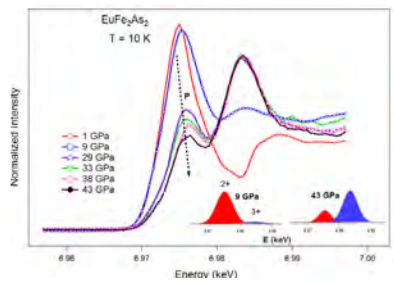


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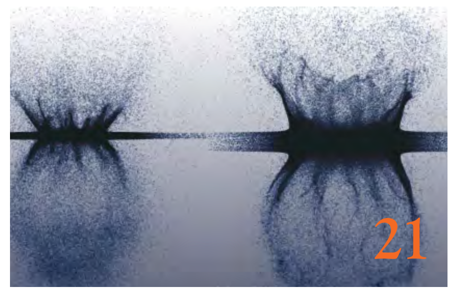


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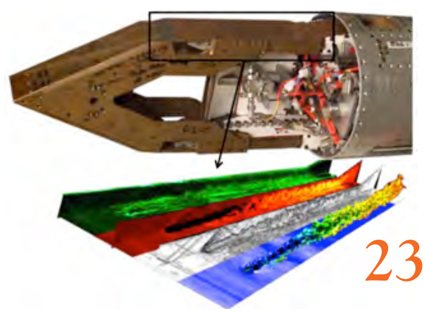

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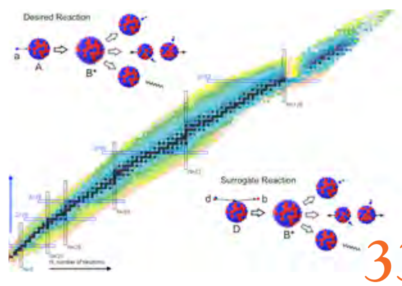


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**Stewardship Science Academic Programs Annual 2013**
*NNSA Office of Stockpile Stewardship*

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Keith LeChien

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

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# Stewardship Science Academic Programs

## Office of Stockpile Stewardship, National Nuclear Security Administration (NNSA)

The mission of the National Nuclear Security Administration's (NNSA) Office of Stockpile Stewardship includes supporting the research and development necessary to guarantee the safety, reliability and effectiveness of the nation's nuclear arsenal, as well as insuring the continued existence of a major component of the nation's nuclear deterrent—the highly skilled and highly regarded scientific and technical workforce at the nuclear weapons national laboratories. As part of the strategy to achieve these mission objectives, the Office of Stockpile Stewardship annually invests resources in university-based programs under the Stewardship Science Academic Programs (SSAP). The SSAP funds research and development across the nation in investigations of relevance to the Stockpile Stewardship Program (SSP) and invests in the training of the next generation of highly skilled individuals for the nation's national security needs.

"This Program is vital to the nation's Stockpile Stewardship Program. Supporting academia in technical disciplines of interest to the stewardship mission enables a strong pipeline of scientists and engineers needed to sustain the nation's nuclear deterrent for decades to come," said Keith LeChien, Stewardship Science Academic Alliances (SSAA) Program Manager.

In this annual report, some of the outstanding work performed under the SSAP is highlighted. The elements of the SSAP include the following: (1) SSAA Program, (2) High Energy Density Laboratory Plasmas (HEDLP) Program; (3) National Laser Users' Facility (NLUF); and the (4) Predictive Science Academic Alliance Program (PSAAP). Each of these Programs has recently solicited new proposals and, after a thorough review process, selected new grant recipients with award periods ranging from one to five years.

Also included as elements of the SSAP, but not highlighted in this Annual, are two programs for outstanding graduate students—the Stewardship Science Graduate Fellowship (SSGF) Program and the Computational Science Graduate Fellowship (CSGF) Program, the latter of which is jointly supported with DOE's Office of Science. These Fellowship Programs provide excellent benefits and opportunities to students pursuing PhDs in areas of interest to stockpile stewardship. For more information about these Fellowship Programs, visit http://www.krellinst.org/fellowships.

### Stewardship Science Academic Alliances Program

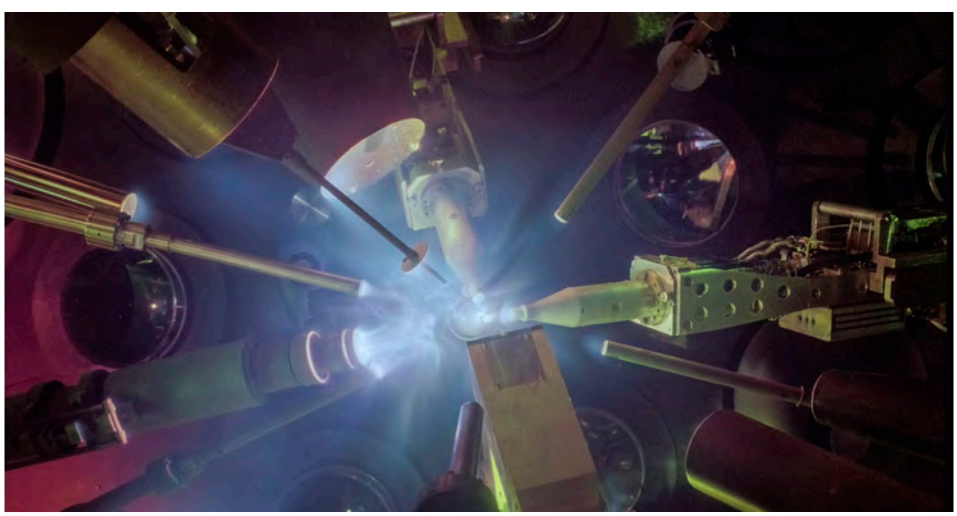
NNSA launched the SSAA Program in 2002 to support research by academic institutions through Centers of Excellence and research grants. The Program emphasizes those areas of fundamental research and development that are relevant to the SSP mission, underfunded by other federal agencies, and for which there is a recruiting need at the NNSA National Laboratories. The goal of the Program is to support advanced experimental activities in the fields of materials under extreme conditions and hydrodynamics; low energy nuclear science; radiochemistry; and high energy density physics. Approximately 117 proposals were received for the 2012 SSAA solicitation. After the review process, awards were given to 40 applicants. In this Annual, we highlight only a few of the outstanding research projects within the Program.

### High Energy Density Laboratory Plasmas Program

The NNSA's Office of Inertial Confinement Fusion and the DOE's Office of Fusion Energy Sciences established the joint program in High Energy Density Laboratory Plasmas in 2008. It involves the study of ionized matter in laboratory experiments where the stored energy reaches approximately 100 billion joules per cubic meter (pressures of approximately 1 million atmospheres). Some of the areas of interest include high energy density hydrodynamics, radiation-dominated hydrodynamics and material properties, nonlinear optics of plasmas and laser-plasma interactions, and warm dense matter. Approximately 185 proposals were received for 147 research projects for the 2012 HEDLP solicitation. After the review process, 46 awards were made. This Annual highlights only a few of the exciting research projects funded by NNSA.

### National Laser Users' Facility Program

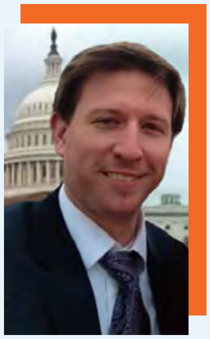
The NLUF was established in 1979 for the primary purpose of providing facility time for university- and business-led



Inside of the OMEGA target chamber during an NLUF experiment led by Paul Drake of the University of Michigan to characterize the spatial temperature profile of a blast wave. Several OMEGA beams drive a blast wave in carbon foam. After a delay of several nanoseconds, a second set of beams irradiates an nickel foil creating an x-ray source for the imaging x-ray Thomson scattering (IXTS) diagnostic. The IXTS is used to measure the spatial profile of this scattering. Timing of the beams was adjusted to to probe the evolution of the blast wave in time.

## Q&As with Dr. Keith LeChien, Stewardship Science Academic Alliances Program Manager

### What is Stockpile Stewardship?



The mission of Stockpile Stewardship is to routinely assess the safety, security, and effectiveness of the nuclear weapons stockpile in the absence of nuclear testing. These assessments are executed by combining new laboratory experimental data with historic data, including nuclear test data, to develop physics-based computer models that are implemented using the world's fastest supercomputers. Stockpile Stewardship is entering its third decade—the U.S. has not tested a nuclear weapon since 1992.

### What challenges face Stockpile Stewardship?

Although the U.S. no longer has the same nuclear posture it did during World War II or the Cold War, the nuclear deterrent remains a vital part of U.S. foreign policy, especially in an increasingly globalized and interconnected world. The U.S. nuclear weapons stockpile is the smallest it has been since the Eisenhower Administration and it will continue to be reduced. It is also the oldest it has ever been. Maintaining a credible nuclear deterrent in the face of these challenges is a huge undertaking ($7 billion annually) that requires a specialized and highly trained workforce and state-of-the-art facilities at the national laboratories and production plants.

### Why should young scientists and engineers pursue a career in Stockpile Stewardship?

Basically—it's just *cool*! What scientist or engineer doesn't want to work on extremely challenging and unique problems at some of the worlds most advanced experimental and computational facilities? Not to mention that there are fewer more interesting and impactful opportunities for a technical career than the stewardship of the U.S. nuclear deterrent. In case that isn't enough, in addition to their primary mission of stockpile stewardship, the NNSA National Laboratories execute a diverse range of programs addressing other national security issues. Simply put, the security of the U.S. and its allies fundamentally relies upon having the best and brightest workforce at its national laboratories.

### You were in middle school at the time of the last nuclear test. How did you become interested in Stockpile Stewardship?

A national laboratory scientist gave a talk about a particular aspect of stockpile stewardship when I was an undergraduate and invited me to visit his lab. I was sold instantly. He later supported my graduate work through a fellowship and hired me when I finished. I continue to be extremely impressed with the dedication, creativity, intelligence and sharpness of laboratory technical staff, as well as the collegial nature and *feel* of the laboratories themselves. They're an awesome and rewarding place to spend your career.

high energy density experiments on the Omega Laser Facility at the University of Rochester's Laboratory for Laser Energetics. Through this program, two of the world's most powerful laser systems, OMEGA and OMEGA EP, are accessible to a broad community of academic and industrial research interests, for use as a tool 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. Twenty-three proposals were submitted in response to the NLUF solicitation, and 13 proposals were selected for the NLUF FY 2013-2014 Program. In this Annual, we highlight four of these grants.

### Predictive Science Academic Alliance Program

In 2008, the Advanced Simulation and Computing Program initiated the PSAAP by establishing five university research Centers. These PSAAP Centers focus on 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. The Centers are located at the California Institute of Technology, Purdue University, Stanford University, the University of Michigan, and The University of Texas at Austin.

### SSAP Annual Review Symposium

Each year, the Office of Stockpile Stewardship conducts a symposium during which the recipients of funding from the SSAP present a talk about their progress. The goals of this symposium are to:

- Highlight accomplishments of the academic programs. These presentations are part of the periodic review of the Program, to assess progress and ensure alignment with Program objectives;
- Promote interaction and help build user communities in areas of physical science relevant to stockpile stewardship;
- Foster ties between participants, sponsors, and the NNSA National Laboratories and identify areas for future collaboration; and
- Encourage student and postdoctoral researcher involvement and interaction with the scientific community.

One of the highlights of this symposium is the poster session which affords the students an opportunity to discuss their research with other attendees, DOE, NNSA, and Laboratory staff. The symposium creates opportunities for students to make connections with others in their field of research that last a life time.

The 2013 SSAP Symposium is scheduled for June 27-28 in Albuquerque, New Mexico. For more information, visit http://www.orau.gov/ssaa2013.

# Exploring Matter Under Extreme Conditions Using Pulsed Power Machines

Cornell University
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The Center for Pulsed-Power-Driven High Energy Density Plasmas at Cornell University is engaged in studies of the dynamics and physical properties of the hot dense plasmas that are produced using 0.4-1.2 MA pulsed power generators. The experiments are supported by the extended magnetohydrodynamics (XMHD) computer code PERSEUS, as well as by the development of new diagnostic methods for high energy density (HED) plasmas, including x-ray Thomson scattering and methods to measure magnetic fields under HED conditions. The Center also focuses on its role in training a new generation of HED research scientists by involving undergraduates and masters degree students, as well as doctoral students, in Center research on HED plasmas and their applications. The Center is now beginning its eleventh year of NNSA sponsorship and, this year, we have five undergraduates and two Master of Engineering (MEng) students as well as six PhD students involved in carrying out Center research. During its first 10 years, the Center engaged approximately 24 different undergraduates, seven MEng students, one Master of Science student and 15 PhD students at Cornell University alone. Partner institutions, Imperial College and the University of Rochester, trained an additional 12 PhD students at least in part under the auspices of Center support. Of those 27 PhD students, eight are employed by the NNSA National Laboratories and one is in the process of being hired.

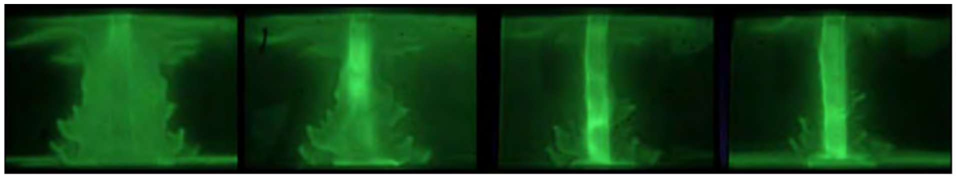

Figure 1. Four 2-ns gated XUV images of an imploding Ne gas-puff z-pinch plasma with 10-ns interframe time. Time goes from left to right. Top of the images is the anode, the z-pinch length is about 2 cm, and there is evidently "zippering" from the anode to the cathode. The 3-mm diameter Faraday rotation cable is visible on the axis. [COBRA pulse #2606]

A major highlight of 2012 was the initiation of gas-puff z-pinch experiments using the tri-axial gas puff valve that was provided to us by Center partner the Weizmann Institute of Science (Israel) on the 1 MA, 100 ns rise time COBRA generator. Experiments were carried out using various gases, including neon which is used in the experiment shown in Figure 1. This pulse also included an applied magnetic field parallel to the gas puff axis to partially stabilize the magneto-Rayleigh-Taylor instabilities. Initial analysis of Faraday rotation and magnetic probe data in these experiments appears to show magnetic field compression as the plasma implodes.

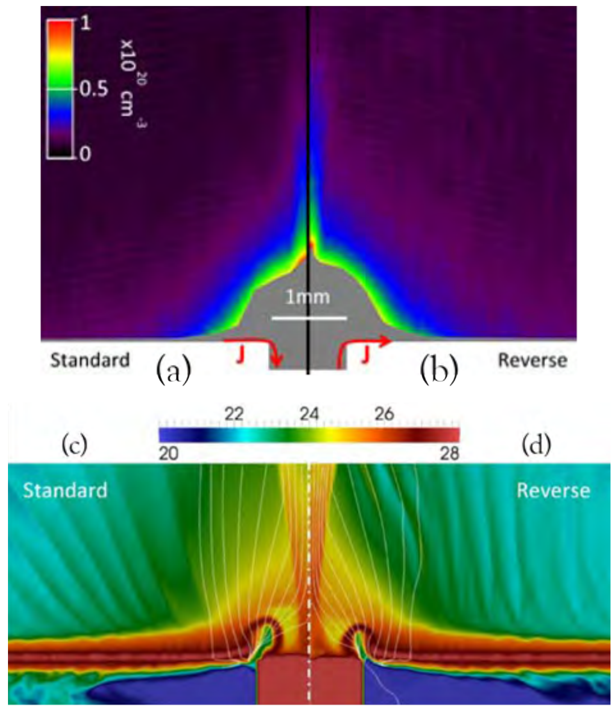


Figure 2. Measured local electron density of (a) COBRA pulse # 02178 with standard electrical current and (b) pulse # 02173 with reverse electrical current are shown compared with the PERSEUS-computed ion density (log10 scale for $m^{-3}$) for (c) standard and (d) reverse currents.

Research using the XMHD code PERSEUS, which includes Hall and electron inertial terms, has continued in 2012. Experimental data have shown that the Hall effect influences directly or indirectly the dynamics and density profile of strongly collimated plasma jets produced from radial aluminum (Al) foils. Comparisons between experiments and PERSEUS simulations indicate that plasma jet properties are modified by the Hall electric field generated in the low-density plasma region surrounding the plasma jet and, therefore, cannot be explained properly by standard MHD. This is shown in Figure 2, in which radially inward plasma flows are larger in reverse polarity (see Figures 2b and 2d) compared to standard polarity (see Figures 2a and 2c). This increase in radial inward flow, which is driven by the Hall effect, is responsible for denser, taller jets observed in reverse polarity.

The success of Sandia National Laboratories' MagLIF inertial confinement fusion concept depends upon achieving an understanding of the physics of liner implosions, in particular plasma instabilities. We have studied liner implosion instabilities with 2-cm-tall, 3-mm-diameter thin Al liners, the pre-test laser image of which is shown in Figure 3a. Laser shadowgraphy shows that instabilities plague the fully imploded liner (see Figure 3b). However, when comparing these data to plasma radiation above 1.2 keV recorded by an x-ray pinhole camera (see Figure 3c), it is clear that the fully imploded liner has developed a kink-like structure. The structure in Figure 3b is evidently trailing mass that has not imploded. Figure

*The Center also focuses on its role in training a new generation of HED research scientists by involving undergraduates and masters degree students, as well as doctoral students, in Center research on HED plasmas and their applications. The Center is now beginning its eleventh year of NNSA sponsorship and, this year, we have five undergraduates and two Master of Engineering (MEng) students as well as six PhD students involved in carrying out Center research.*

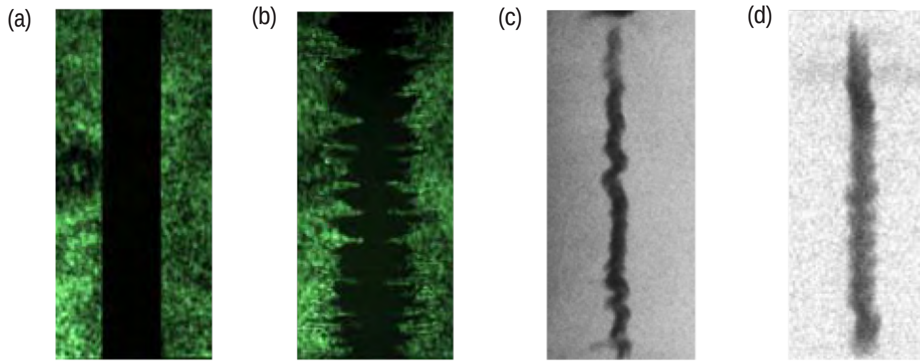


Figure 3. Laser shadowgraph of the liner a) before the shot and b) when fully imploded at t = 150 ns. Time integrated x-ray pin hole camera images with lower energy cutoff at 1200 eV with no applied B field for c) shot # 02575, and with an applied B field for d) shot # 02614. The total height of the liner is 2 cm, its diameter is 3 mm.

Figure 4. Post doctoral associate Kate Blesener, undergraduate student Elliot Rosenberg, and graduate students Cad Hoyt and Peter Schrafel insert and level an x-ray spectrometer in the COBRA vacuum chamber for high energy density z-pinch experiments.

3d shows that when a 1 T axial field is present, the plasma instabilities are different and the column radius appears to be larger at full compression.

Thin radial Al foils have been tested on COBRA in a variety of configurations of the central cathode (Figures 2a and 2b have a single central cathode), which changes the ablation pattern on top of the foil. Perturbing the ablation pattern with applied axial magnetic fields (up to 1.3 T) tends to decrease azimuthal perturbations of the ablation pattern and to cause the jet to be more hollow than it would be without an applied field. Understanding the plasma dynamics from ablation of the foil to jet formation with and without the applied field is vital to establishing the relevance of these jets to astrophysical observations.

Many diagnostics are used on each experiment, not just those discussed here. In order to obtain plasma conditions, for example, in experiments such as the ones shown in Figures 1, 2, and 3, we make use of both visible spectroscopy for lower temperature plasmas and with Bragg crystal x-ray spectroscopy for higher temperature plasmas, as shown in Figure 4.

# Continuation of the Application of Particle-in-Cell Simulations to Laser and Electron Transport Through High Energy Density Laboratory Plasmas

University of California, Los Angeles
PI: Warren B. Mori, mori@physics.ucla.edu

The University of California, Los Angeles (UCLA) Simulation of Plasmas Group http://plasmasim.physics.ucla.edu has been supported by the NNSA for over a decade to carry out research on laser and energetic particle transport in high energy density plasmas. These processes are fundamental research topics in the area of the nonlinear optics of plasma, as well as being directly relevant to inertial fusion energy. The Group studies these processes with computer models that can run effectively on the largest computers in the world. The study of the nonlinear optics of plasmas, as well as high performance computing, attracts talented graduate students and post doctoral researchers.

Over the years, the NNSA funding has supported the training of seven graduate students and three post doctoral researchers. A current student is now a Lawrence Scholar at Lawrence Livermore National Laboratory (LLNL). One graduate student who was partially supported is now at Los Alamos National Laboratory, another is at a private company working in the defense industry, while others have continued working in the field as post doctoral researchers. One post doctoral researcher became a faculty member at the University of Rochester. In addition, courses developed as part of this research are also taken by experimental students, two of whom are at LLNL. This program and its annual symposium have a tremendous benefit to the education and training of graduate students, as it allows them to understand the quality of research and opportunities at the nation's national laboratories and to see the national significance of their research.

The Group continues to develop and use its state-of-the-art simulation tools to understand how a laser interacts with a high energy density plasma. This is critical for the success of the National Ignition Facility and for inertial fusion energy, and it is of fundamental importance to the nonlinear optics of plasmas.

In laser driven inertial fusion energy, it is imperative that laser light reaches where it is aimed. A high energy density plasma can scatter light, bend laser light, and transfer the light energy into energetic electrons. This occurs because a laser propagating in plasma can effectively couple to plasma waves through instabilities named stimulated Raman scattering, two-plasmon decay, and the high-frequency hybrid instability. These are extremely complicated processes because they involve waves coupling to waves, particles surfing on waves, and the highly dispersive nature of plasma waves. Due to the complexity of these interactions, computer simulations that follow the individual trajectories of plasma particles are necessary to make sense of it all.

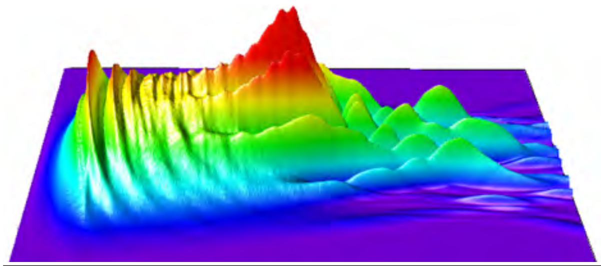

Figure 1. Finite-width nonlinear plasma waves are subject to transverse localization and filamentation. Shown is the temporal evolution of a finite-width, nonlinear electron plasma wave (transverse profile of longitudinally-averaged field energy). Results of a two-dimensional UPIC simulation.

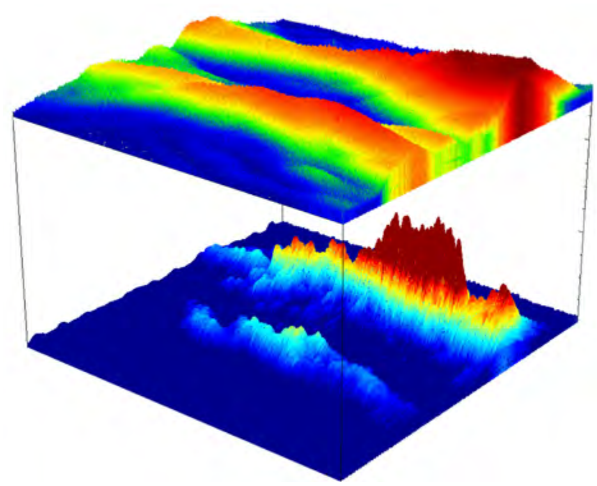

Figure 2. Stimulated Raman scattering (SRS) can be triggered in below-threshold laser speckles by scattered waves and particles traveling into it from SRS in neighboring speckles. Shown here are two laser speckles (top plane) and SRS-generated plasma waves (bottom plane). Scattered light from the above-threshold speckle (in the region with highest amplitude EPW signal) stimulates SRS activity in the below-threshold speckle (region with lower amplitude EPW signal).

The UCLA Group uses what are called particle-in-cell (PIC) models to study these processes. Using its own massively parallel PIC codes, it has studied how multi-dimensional plasma waves evolve due to how a small subset of particles give and take energy out of the wave. This is shown in Figure 1. The Group has continued to study how higher than expected electron energies can be generated when laser light is reflected off plasma waves. The very energetic electrons arise when the laser scatters both backward and forward and when this scattered light re-scatters, generating a spectrum of plasma wave packets. Electrons first surf on the slower wave and then progressively bootstrap their way onto the faster waves. The UCLA codes have also been used to study how individual packets of laser energy can mutually interact. When one laser packet is scattered from stimulated Raman scatter, it can trigger another nearby (or far away) packet from scattering. This can be achieved by either the reflected laser light moving through another packet or the energetic electrons produced inside one packet moving into another. The group has isolated these effects and clearly shown that both can occur. An example is shown in Figure 2.

# Z-pinch Research on Radiation, Atomic and Plasma Physics

University of Nevada, Reno
PIs: Alla S. Safronova, alla@unr.edu and Victor L. Kantsyrev, victor@unr.edu

The rapidly advancing field of high energy density physics as a frontier science incorporates many different subdisciplines. Since 2006, we have been supported by NNSA and made it a priority to train students in radiation, atomic and plasma physics to contribute in creating the future workforce needed by NNSA laboratories, and to advance in *z*-pinch physics and relevant subdisciplines. During the last six years, 10 graduate students have been supported; five graduate students and three undergraduate students were involved in this research during 2012. From our recently graduated students, Kenneth Williamson began working for Sandia National Laboratories (SNL) in 2012 and Nicholas Ouart continues his second year at the Naval Research Laboratory.

The year 2012 was very productive. Twelve papers were published, five of which were authored by current and former graduate students. In particular, graduate student Michael Weller published his research on radiative properties of mixed nested cylindrical wire arrays in collaboration with SNL and interdisciplinary research on extreme ultraviolet (EUV) spectroscopy and modeling of copper on the Spheromak and the compact laser plasma facility in collaboration with Lawrence Livermore National Laboratory. Graduate student Glenn Osborne completed his PhD studies on investigations of tungsten-based *z*-pinch planar wire arrays, and two undergraduate students earned their physics degrees.

The increase in current from 1 MA to 1.7 MA on the university-scale *z*-pinch generator Zebra at the University of Nevada, Reno (UNR) has allowed for experiments with implosions of larger sized wire arrays. These have provided enhanced energy coupling in plasmas and better diagnostics access. In particular, the results of the recent simulations and experiments with multi-planar wire arrays (PWA) from outer planes made from nickel (to create an effective L-shell radiator) placed at the larger distance and half-empty middle aluminum (Al) plane (to create K-shell Al plasma that will influence radiation from outer planes) are highlighted in Figure 1. They represent an excellent set of data to advance the subdisciplines of radiation physics (how the mixture of two plasmas radiate), plasma physics (why a hot precursor was formed that was never observed before in PWAs), and laboratory astrophysics (how plasma flow is affected by the initial internal magnetic field and what is the nature of observed standing shocks).

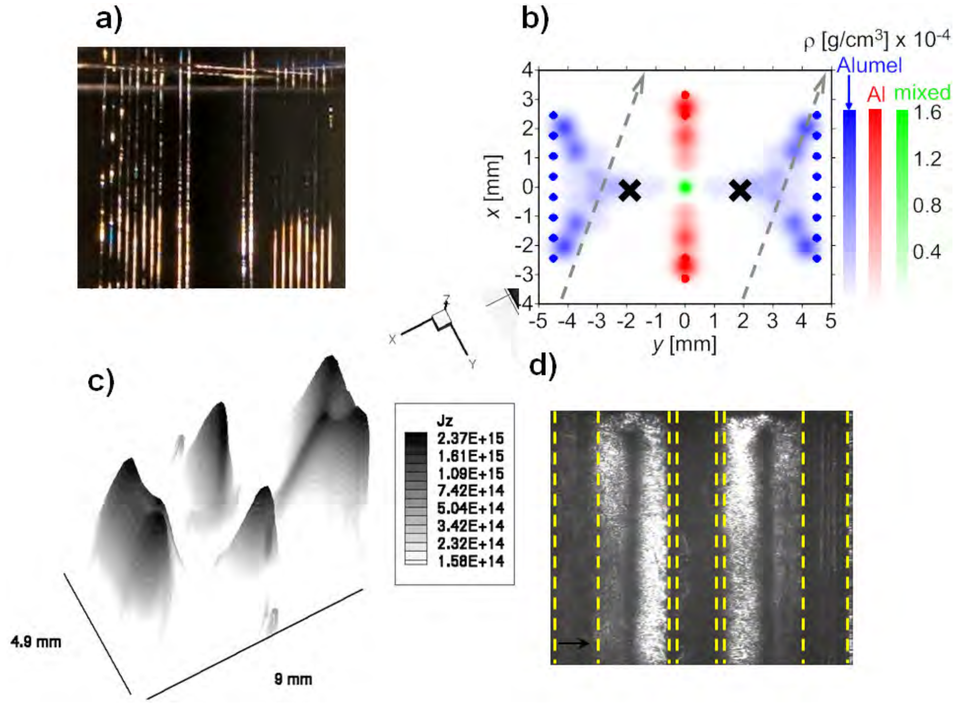


Figure 1. Implosion of the larger size planar wire arrays at 1.7 MA Zebra at UNR. a) Photograph of Triple Wire Array load. b) Wire Ablation Dynamic Model predictions at 60 nsec (view from the top). Dotted arrowed lines show the direction of optical laser probing. c) Two-dimensional radiation magnetohydrodynamic calculation of the current profle at 70 ns by the collaborator, Dr. A. Chuvatin (Ecole Polytechnique). d) Shadowgraphy image at 61 ns. Column-like structure between wire planes on the laser shadow images is likely the standing shocks that change the direction of ablated plasma flows (marked by black crosses on the above map). Yellow dotted lines show the initial positions of wires. Time is counted from the start of the current.

The study of a new compact hohlraum configuration with PWA sources, unique for university-scale generators, continues on Zebra. Magnetically insulated double PWA sources in cages showed well-synchronized implosions and x-ray bursts. A numerical simulation capability using VisRaD (from PRISM company) code established at UNR allowed the study of hohlraum coupling physics and the possibility of its design optimization. The radiation temperature $T_R$ of the hohlraum central cavity with re-emission target was measured using cross-calibrated filtered EUV Si-diodes. Experimental $T_R$ (from 42 eV to 55 eV) was in favorable agreement with $T_R$ = 38 eV from the simulation. The first results of theoretically optimizing a new compact hohlraum indicated $T_R$ increased by 1.15 times and x-ray power flux increased by 1.7 times.

Though selected topics mentioned above constitute two important directions of our studies, during the last year our research on Z-pinch physics was broader and included more topics that were developed and presented at four conferences and a symposium.

# Center for Excellence for Radioactive Ion Beam Studies for Stewardship Science

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Low energy nuclear physics is one of the forefront areas of modern science that is helping us to understand fundamental questions such as the origin of the elements in the cosmos. Low energy nuclear science can also provide solutions to some of the challenging problems facing our nation by developing passive and active nuclear detection systems for homeland security. Research activities in this field train the next generation of leaders in fundamental research and in applications of low energy nuclear science, from nuclear forensics to homeland security to nuclear energy.

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. The focus has been to use radioactive ion beams of fission fragments and other rare isotopes to study reactions on, and structure and decay of, atomic nuclei far from stability. Studies with many of these short-lived isotopes can help us understand the origin of the elements. These efforts require new theoretical approaches, new experimental tools and new rare isotope beams. Realization of these research efforts requires a highly talented team that includes graduate students and post doctoral scholars.

In the fall of 2012, eight graduate students and five post doctoral researchers are supported at least in part to play important roles in research efforts of the RIBSS. They are included in the total of 26 graduate students and 18 post doctoral researchers since 2003. In addition, 36 undergraduates have been supported by the Center, with five receiving at least partial support in 2012 from SSAA funds. Three alumni of the RIBSS are staff members at Lawrence Livermore National Laboratory (LLNL) and two are post doctoral researchers at LLNL and Los Alamos National Laboratory (LANL), respectively. In addition, one alumnus is a staff member at Oak Ridge National Laboratory (ORNL) and two are faculty members at research universities, who, along with their students and post doctoral researchers, continue to work with the RIBSS.

The SSAA funds have enabled a synergistic collaboration of low energy nuclear scientists at five universities and two national laboratories to educate early career nuclear scientists, develop new instruments, and enhance connections with nuclear science efforts at LLNL and LANL.

## Research Highlight: Deducing Neutron Capture on Neutron-rich Tin Isotopes

Nuclear reactions in which a neutron is captured by an atomic nucleus are responsible for the synthesis of almost all of the elements heavier than iron. Neutron-induced reactions also generate the energy in nuclear reactors and in nuclear devices. The rapid neutron capture r-process that occurs in extremely high neutron fluence explosions in the cosmos proceeds through nuclei far from stability with very short half-lives. Many of the slow s-process captures also occur on unstable nuclei. The ability to measure neutron capture on unstable nuclei is limited. Even the Detector for Advanced Neutron Capture Experiments at LANL is restricted to studies of nuclei with half lives greater than about 100 days. Therefore, new techniques to measure neutron capture probabilities or cross sections on unstable atomic nuclei need to be developed.

The RIBSS Center has been a world leader in exploiting radioactive ion beams of fission fragments to measure nuclear reactions in which a neutron is transferred from the target to the beam. Recent studies with $^{130}$Sn beams are a key example. The lack of knowledge of neutron capture cross section on $^{130}$Sn limits the accuracy of predictions of r-process nucleosynthesis over a wide range of nuclear masses, both below and above the mass 130 region.[1,2] Uncertainties in the $^{130}$Sn neutron capture cross sections could also affect calculations of energy production in reactors and nuclear devices. Direct capture is an important component of the neutron capture on $^{130}$Sn. Prior to our studies, uncertainties in direct capture cross sections varied by three orders of magnitude.[2]

To inform neutron capture on $^{130}$Sn required beams of this short-lived fission fragment ($t_{1/2}$= 3.7 min) interacting with deuterated polyethylene $CD_2$ targets (the nucleus of deuterium, heavy hydrogen, consists of a neutron and a proton). The beams were produced at the Holifield Radioactive Ion Beam Facility at ORNL, where protons induced fission of $^{238}$U and the mass-separated $^{130}$Sn fission fragments were accelerated to 630 MeV. The $^{130}$Sn ions stripped a neutron from the deuterium in the target; the resulting proton was detected in an early implementation of the Oak Ridge Rutgers University Barrel Array (ORRUBA) of position-sensitive silicon strip detectors that was constructed with SSAA funds and is displayed in Figure 1. The Q-value spectrum of the reaction protons that populate states in $^{131}$Sn is displayed in Figure 2. The energy and intensity of the peaks corresponding

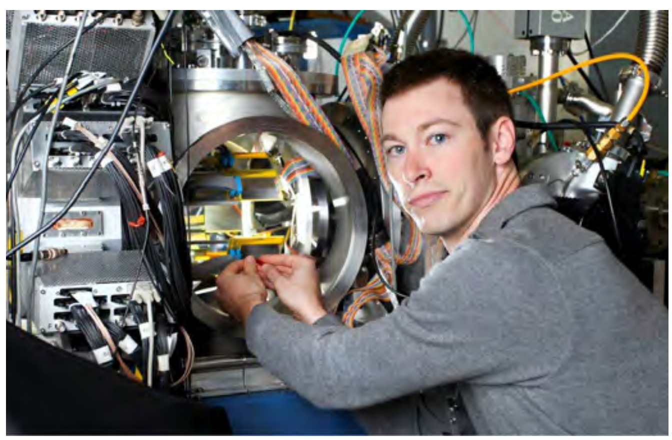

Figure 1. Photograph of ORRUBA detectors with SSAA-supported graduate student Brett Manning.

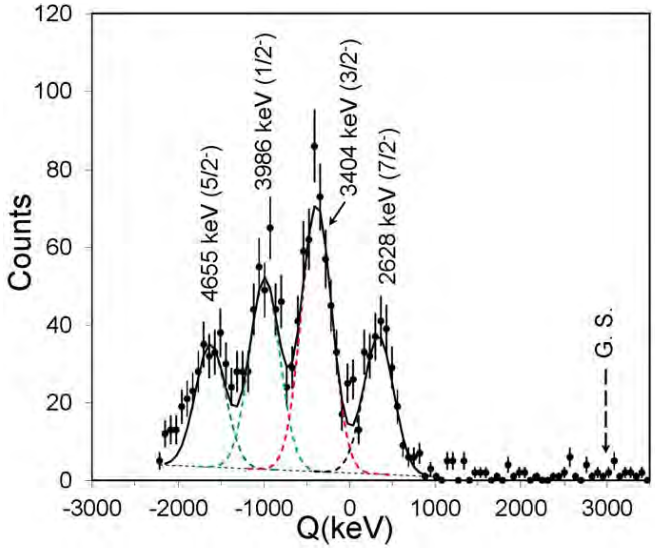


Figure 2. Q-value spectrum of protons measured with an ORRUBA detector from the (d,p) reaction with radioactive ion beams of $^{130}$Sn. The peaks are labeled with approximate $^{131}$Sn excitation energies and tentative spin and parity values. The $\ell$=1 transfer to the tentative 3/2$^-$ and 1/2$^-$ states are most important for direct neutron capture. Adopted from reference 3.

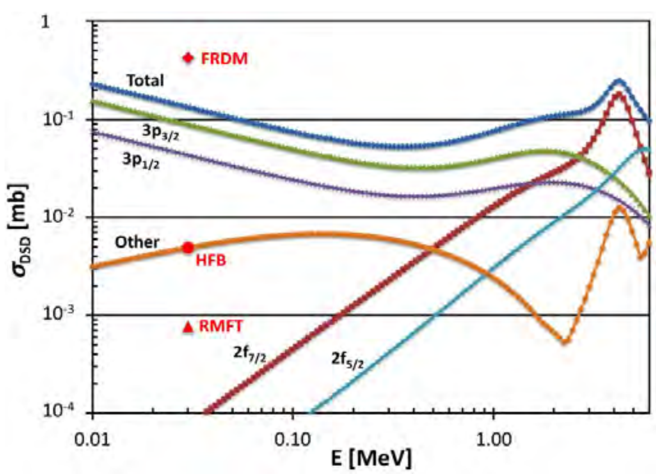


Figure 3. Calculations of cross sections for direct-semi-direct neutron capture on $^{130}$Sn as a function of neutron energy in MeV. Present calculations are compared to previous ones[2] at $E_n$= 30 keV for three different models of nuclear masses. Adopted from reference 3.

*The SSAA funds have enabled a synergistic collaboration of low energy nuclear scientists at five universities and two national laboratories to educate early career nuclear scientists, develop new instruments, and enhance connections with nuclear science efforts at LLNL and LANL.*

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to orbital angular momentum $\ell$=1 transfer to $^{131}$Sn are most important for neutron capture and were used as input in calculating the direct neutron capture cross section, summarized in Figure 3, and in significantly reducing the uncertainties in predicting neutron capture on $^{130}$Sn. Recent measurements[4] have extended these studies to the neutron-rich $^{126,128}$Sn isotopes; the results are under analysis.

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# Detecting Low-Energy Fission Neutrons

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The spectrum of prompt neutrons released in the fission process spans a wide range of energies. Typically, about 30% of this yield occurs below 1 MeV. Difficulties in reliably detecting these relatively low energy neutrons have led to a dearth of direct measurements of the relevant fission neutron yields. Experimentally, the problem derives from the gamma-ray backgrounds which cannot be distinguished from low energy neutrons by the usual techniques of pulse shape discrimination.

With support from the Stewardship Science Academic Alliances (SSAA) Program, a novel method has been developed for obtaining fission neutron time-of-flight spectra with a large-acceptance scintillation detector optimized for neutrons below 1 MeV. The detector design is intrinsically capable of rejecting gamma-ray backgrounds with high efficiency, and does not rely on pulse shape differences between gammas and neutrons. This work is carried out at the University of Kentucky by the principal investigator and two graduate students using neutron beams produced both with the local accelerator, as well as at the Los Alamos Neutron Science Center (LANSCE) facility at Los Alamos National Laboratory (LANL). Currently, the group is in the third year of their work.

SSAA support for this project has been crucial in allowing our students to work side-by-side with LANL scientists in helping to resolve an important gap in our knowledge of the fundamental process of nuclear fission.

The detector uses 100-cm-long strips of plastic scintillator, each with a thickness of only 3 mm. Ten layers of these strips are sandwiched together, and light from each stack of five alternate layers is combined and read out with photomultiplier tubes. In Figure 1, the students are seen with the disassembled detector. The active region of scintillator is flared into Y-shaped light guides where the photomultipliers are attached.

When low energy neutrons scatter from free protons in the detector, the protons recoil a very short distance and produce scintillation light. Low energy gamma rays, on the other hand, interact to produce recoiling electrons whose range is typically several millimeters—large enough to create scintillation light in pairs of adjacent detector layers. Gamma rays are distinguished from neutrons according to whether adjacent layers did or did not trigger. Figure 2 shows the detector's response to a gamma-ray source, and its measured efficiency of gamma-ray rejection.

A pair of layered detectors will be used at LANSCE in early 2013, to observe neutrons produced in coincidence with fission fragments following neutron-induced fission in a uranium target.

Figure Caption 1. The individually wrapped scintillator layers, and their Y-shaped light guides.

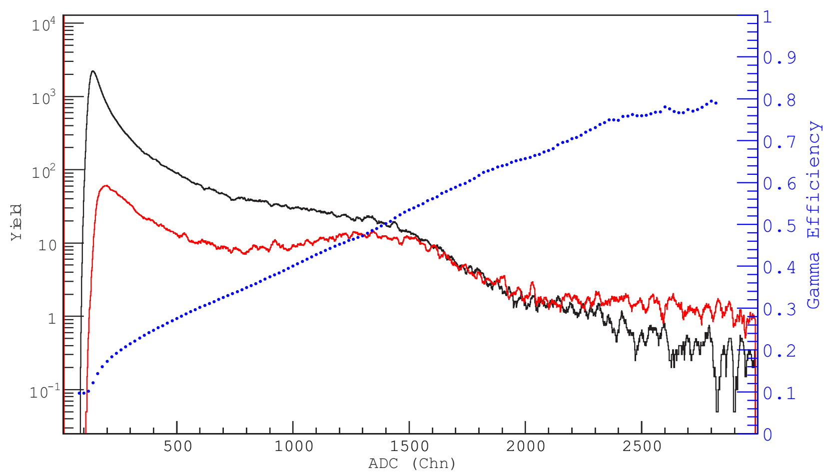


Figure 2. Measured pulse-height spectra for a Co-60 gamma-ray source. The red curve shows events in which adjacent layers of scintillator were triggered, indicating a gamma-ray event. The black shows events in which only one layer of scintillator was triggered. The blue curve gives the integral efficiency for identifying gamma rays as a function of the lower threshold energy.

# Theoretical Description of the Fission Process

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Advanced theoretical methods and high-performance computers may finally unlock the secrets of nuclear fission, a fundamental nuclear decay that is of great relevance to society. Since 2003, the nuclear theory group at the University of Tennessee has studied the phenomenon of nuclear fission using the symmetry-unrestricted nuclear density functional theory (DFT). The aim is to replace current phenomenological models with a microscopic theory that delivers maximum predictive power with well-quantified uncertainties. The program currently supports two graduate students. Three former students, one now a post doctoral researcher at Lawerence Livermore National Laboratory (LLNL), received their doctorate degrees under this program.

Currently, the major component of their support comes from the Stewardship Science Academic Alliances (SSAA) Program. This grant provides indispensable support for students, post doctoral researchers, and visitors working on fission theory. In particular, it has enabled the University of Tennessee, Knoxville (UTK) group to train junior scientists and students to apply nuclear many-body techniques to describe low energy nuclear phenomena. The SSAA-funded research greatly benefits from the Scientific Discovery through Advanced Computing program of DOE's Office of Advanced Scientific Computing Research that provides algorithmic and numerical help and extensive computational resources involving petaflop platforms and beyond. Extreme-scale computing affords the researchers the opportunity to relax assumptions, so that they can calculate fission properties with increasing fidelity, and therefore enables validation with experiments.

The phenomenon of induced nuclear fission, the splitting of a heavy atom by a neutron into two smaller atoms, was discovered more than 70 years ago. In 1939, Niels Bohr and John Archibald Wheeler developed a macroscopic theory of fission. A year later, the experimental evidence for spontaneous fission, a form of radioactive nuclear decay, was obtained. Today, a comprehensive microscopic explanation of nuclear fission rooted in interactions between protons and neutrons, the building blocks of the atomic nucleus, still eludes us. This is an example of a quantal collective motion during which the nucleus evolves in a multidimensional space representing shapes with different geometries, going through regions that are forbidden by classical mechanics. Because of the complexity of the process, we have yet to obtain a microscopic picture of fission that is of comparable quality to that for ground and excited states of atomic nuclei.

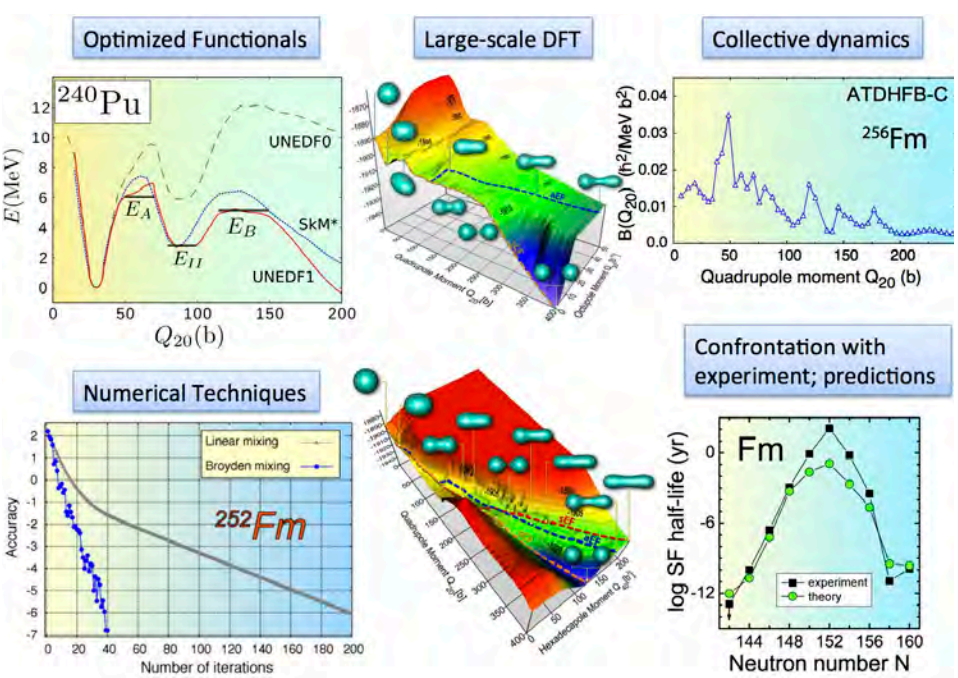


Figure 1. Theoretical approach to fission. Calculations use quality density functionals optimized for large deformations, such as UNEDF1 (upper left) and state-of-the art numerical techniques (lower left). Large-scale DFT calculations in multidimensional collective spaces are needed to produce accurate potential energy surfaces, which enable us to identify the multiple fission channels (middle). Large-scale dynamical simulations (upper right) calculate fission lifetimes, fission fragment properties, and other observables (lower right).

The microscopic description of fission represents an extreme-scale application of the nuclear DFT (see Figure 1). The quality of simulations depends on microscopic input, e.g., the deformability of the energy functionals. A significant effort has been devoted to develop energy functionals that produce the correct physics at large shape elongations and develop numerical techniques and tools that would facilitate symmetry-free constrained DFT calculations. A starting point in the adiabatic approach to fission is to compute accurate multi-dimensional potential energy surfaces, and use them to compute observables such as fission half-lives or fragment distributions. Results obtained along one-dimensional trajectories are very encouraging. More precise theory will require a full treatment of the collective inertia tensor and the direct minimization of the collective action in a multidimensional collective space.

An improved understanding of the microworld benefits society and fission is an example in which theoretical progress will have practical consequences. Given the encouraging results to date and the recent developments of powerful conceptual and computational tools for nuclear structure modeling, one is optimistic that we may be very close to understanding this fundamental process.

## Research and Educational Efforts at the High Pressure Science and Engineering Center (HiPSEC)

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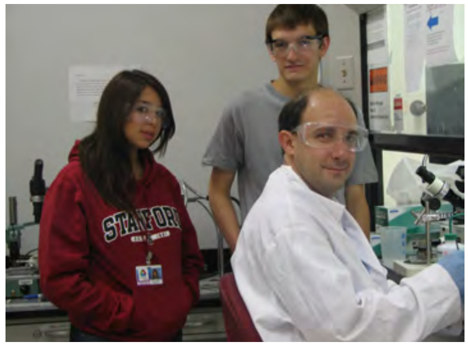
The High Pressure Science and Engineering Center (HiPSEC) at the University of Nevada, Las Vegas (UNLV) was founded in 1998 through the collaboration between the UNLV and the NNSA to serve as a university-based teaching and research center to support NNSA's Stockpile Stewardship Program (SSP). The Center has since established a multi-disciplinary research program focusing on fundamental experimental and computational studies of material properties at extreme conditions. HiPSEC has also devoted many resources to educational and outreach efforts to train the next generation of scientists. The Center currently supports 12 graduate students (seven PhD and five MS) and 26 undergraduate students. In addition, HiPSEC hosts seven to 10 students from UNLV's summer Research Experiences for Undergraduates Program each year. These students are recruited from universities and colleges around the country. More than 250 students have been supported by HiPSEC since its inception. Students at all grade levels are encouraged to seek opportunities in various government agencies and national laboratories. One HiPSEC-supported student, Zachary Quine, worked at the Army Research Laboratory in Aberdeen Proving Ground for one year and subsequently received a Science, Mathematics and Research for Transformation (SMART) fellowship. Another undergraduate student who continued his graduate study at the Center and received his master's degree, Edward Romano, is currently working at Lawrence Livermore National Laboratory as a contracted scientist. Jason Baker, a UNLV PhD student, is currently working with Los Alamos National Laboratory (LANL) scientists on SSP materials and has already spent one summer at LANL. Martin Galley came to UNLV as a National Science Foundation Research Experiences for Undergraduate (NSF-REU) summer student and continued at UNLV as a masters student supported by HiPSEC. He has successfully completed the MS program and is now a commissioned officer with the U.S. Navy receiving nuclear submarine operational training. Current graduate student, John Howard, is stationed at LANL as a Graduate Assistant; he is collaborating with LANL scientists for his PhD research projects.



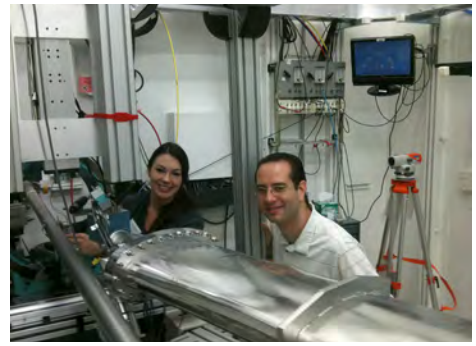


Figure 1. Left - Dr. Pravica loading hydrazine in a diamond anvil cell with his students, Mai Bausch and John Robinson, at HPCAT's sample preparation facility at APS. Right - PhD students Daniel Antonio and Elizabeth Tanis setting up inelastic x-ray scattering (IXS) measurement at sector 3 of APS.

HiPSEC scientists have created a group of web-based educational modules about high pressure science topics. Potential users of the modules include faculty, undergraduates and graduate students. An online course entitled "Introduction to Mineral Physics" has been taught during the spring 2012 semester. More than 20 students and post doctoral researchers as well as 15 faculty and senior scientists participated in the course. The modules reside in the *On the Cutting Edge*, Teaching Mineralogy collection on the Science Education Resource Center website: http://serc.carleton.edu/NAGTWorkshops/mineralogy/mineral_physics/index.html.

NNSA funding is vital to the collective effort within HiPSEC to bring together physicists, chemists, geoscientists and engineers to work on cutting-edge problems central to the SSP interests. More importantly, support from NNSA enables tremendous exposure of national security sciences to a generation of future scientist, as large numbers of students of all grade levels are actively involved in HiPSEC's research and educational activities.

"My research and ability to involve students in my research have been greatly enabled via funding from the NNSA. In addition, NNSA's strong support of the High Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source (APS), of which HiPSEC is a founding member, has been a tremendous factor in inspiring my students to go even further in science, garner critical skills to aid them in their future careers, and to better understand the NNSA mission," said Dr. Michael Pravica, one of UNLV faculty supported by HiPSEC (see Figure 1).

### Research Highlights

HiPSEC and UNLV scientists collaborated with those at LANL in fabricating a sample cell assembly for *in situ* thermal conductivity, resistivity, Seebeck co-efficient, and structural measurements using the Paris-Edinburgh type large volume cell located at 16-BMB station of HPCAT, APS. They have successfully performed the transport and structural measurements by studying the *P-T* phase diagram of bismuth up to 6 GPa. This setup allows simultaneous measurement of thermal, electrical and structural parameters for a variety of technologically important intermetallic systems.

The interplay between pressure and superconducting transition temperature, valence, spin fluctuations, magnetic ordering and crystal structure are not well understood. $EuFe_2As_2$ belongs to the recently discovered iron-pnictide family of superconductors. The compound undergoes a magnetic and structural transition below 190 K at ambient pressure. Suppression

*"...NNSA's strong support of the High Pressure Collaborative Access Team at the Advanced Photon Source, of which HiPSEC is a founding member, has been a tremendous factor in inspiring my students to go even further in science, garner critical skills to aid them in their future careers, and to better understand the NNSA mission."*

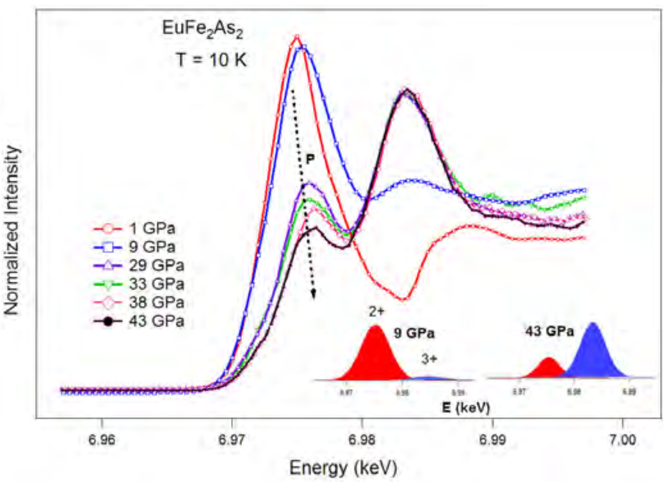



Figure 2. X-ray absorption in Partial Florescence Yield mode collected at 10 K for various pressures. The spectra clearly show the divalent to trivalent transition of Eu under high pressures at low temperature.

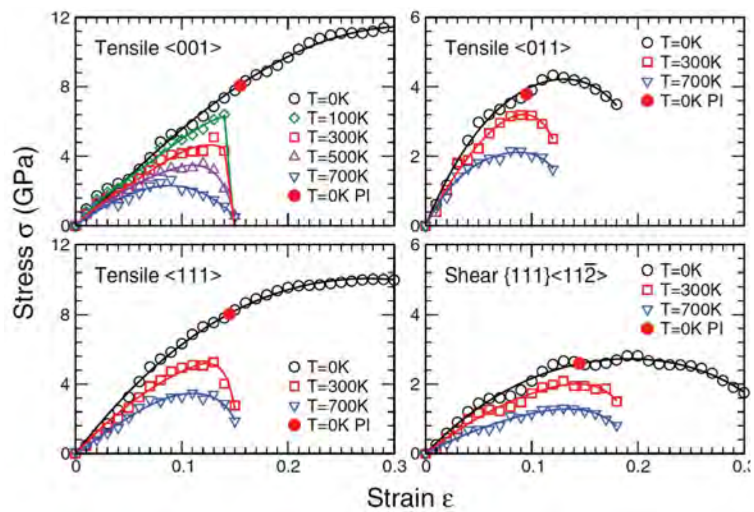



Figure 3. The calculated average stress-strain relations of aluminum under various tensile and shear deformation directions at T = 0 K, 300 K, and 700 K.

of spin density waves and evolution of superconductivity were observed under pressure above 2.8 GPa. It is important to understand the valence and magnetic moments of $Eu^{2+}$ near the superconducting transition. Resonant inelastic x-ray scattering is a sensitive probe to study the electronic structure of solids. Unlike photoemission, it is bulk sensitive and element specific. HiPSEC scientists have used this versatile technique to study and demonstrate pressure induced valence change of Eu under high pressures at low temperature in $EuFe_2As_2$ (see Figure 2).

Scientists at HiPSEC have harnessed the hard x-rays at APS to perform acatalytic *in situ* chemistry in isolated and/or extreme conditions and with little or no addition of heat. A novel method has been developed to load sealed enclosures (such as the diamond anvil cell) with difficult-to-load molecular gases (such as hydrogen). Phase-dependent decomposition has been discovered in potassium chlorate and other materials wherein the radiation-induced decomposition rate varies with phase and thus, pressure. This has enabled the ability to slow or speed the decomposition of molecules as well as to control molecular mobility within the isolated chamber. Finally, an energy-dependence to the decomposition rate which may negate the need for high flux synchrotron sources has been recently observed.

The origin of different degrees of sensitivity of α-RDX (research department explosive) synthesized using various methods has been much debated. A plausible explanation is the presence of impurities of highly sensitive δ-HMX epitaxially grown on α-RDX crystallites. Using the high-resolution powder diffractometer at the high-flux wiggler beamline X14A at National Synchrotron Light Source, HiPSEC scientists have examined batches of insensitive (i-) and *reduced sensitivity* (rs-) α-RDX with an ~0.1 mass % detection limit. It has been found that rs-RDX contains strained β-HMX inclusions, which have not been detected in i-RDX. It is suggested that the higher sensitivity of rs-RDX is related to the presence of these β-HMX inclusions: local strain at the interfaces between the two coexisting phases is expected to increase upon dynamic compression and plausibly contributes to the conditions for generating hot spots.

Accurate prediction and analysis of material strength and stability is fundamentally important in material science. Based on first-principles molecular dynamics method, scientists at UNLV and HiPSEC have developed a new algorithm that enables the calculation of ideal strength and dynamical stability at finite temperature. This new approach also allows a full relaxation of the crystal structure with respect to the external stress tensor. Application to aluminum (Al) metal reveals that dynamic phonon instabilities under uniaxial tension and shear deformation predicted at T = 0 K are stabilized by thermodynamics at or above room temperature (see Figure 3). Rising temperature also induces significant reduction in the magnitude of the ideal strength and makes the tensile strength of Al much more isotropic. These large-strain calculations can be extended to high-pressure loadings and open a new venue for simulations of material deformation and strength at extreme conditions.

# Experimental Study of the Turbulent Development of Rayleigh-Taylor and Richtmyer-Meshkov Instabilities

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Our group has had a 20-year collaboration with the NNSA, its predecessor, and the NNSA National Laboratories. During this time, 25 students and three post doctoral researchers have engaged in research projects associated with this collaboration and, of these, one has gone on to work at one of the NNSA laboratories. In addition, the Stewardship Science Academic Alliances Program currently supports three graduate students and one post doctoral researcher.

Our research focuses on two important instabilities that occur when an interface separating two unequal density fluids is accelerated. Rayleigh-Taylor instability (RTI) occurs when the system is subjected to constant acceleration and Richtmyer-Meshkov instability (RMI) occurs when the system experiences impulsive acceleration, often produced by a shock wave. These instabilities are of interest to the NNSA as they are important to implosion processes such as those in inertial confinement fusion.

The RTI is studied in a 3-m-tall drop tower that employs a weight and pulley system to accelerate a tank containing two liquids downward at a rate greater than gravity. Initially, the system is stably stratified by gravity. However, the downward acceleration results in a net upward gravitation force producing an unstable configuration in which RTI develops.

One of the primary objectives of this study is to investigate the effects of initial conditions on the resulting turbulent flow. Two types of interfacial initial perturbations are used. The interface is either unforced, where small random perturbations resulting from background noise act as the seed for the instability, or forced, where small wavelength initial perturbations are created by vertically oscillating the tank.

Figure 1 shows a comparison of images obtained from forced and unforced experiments. Note that the forced experiments have a larger mixing layer width than their unforced counterparts.

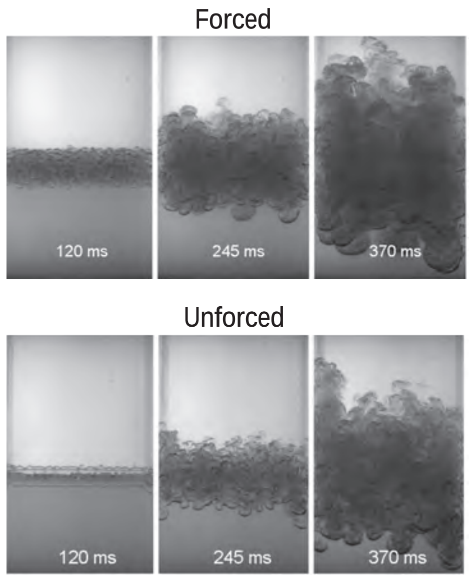


Figure 1. A comparison of RTI experiments with forced and unforced initial perturbations.

However, the non-dimensional growth constant $\alpha$ obtained from these experiments is essentially the same indicating that it is unaffected by the initial perturbation.

The RMI is studied using a low Mach number vertical shock tube consisting of a pressurized driver section that is separated from the driven section by a polypropylene membrane. The experiment is initiated by the puncturing of the membrane, forming a shock wave that travels downward and impacts an interface between a light gas (air) and a heavy gas ($SF_6$) resulting in an impulsive acceleration that drives the instability. A single-mode initial perturbation is generated on the interface by oscillating the shock tube horizontally to produce a sinusoidal standing wave.

The resulting instability is recorded by illuminating smoke particles seeded in the air with a laser light sheet and recording the resulting images using high-speed video photography. Figure 2 shows an image sequence comparing experimental images with those obtained from a simulation obtained using the Lawrence Livermore National Laboratory fluid dynamics code Miranda. One important outcome of this study is that good agreement with simulations can be obtained only if boundary layers that form on the shock tube walls are accounted for in the simulations.

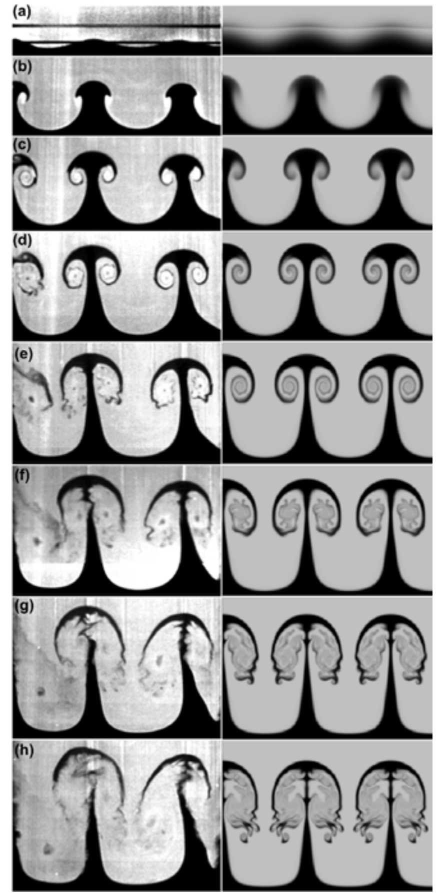


Figure 2. A comparison of a single-mode RMI experiment with simulation where time varies from (a) t=0.08 ms to (h) t=10.42 ms.

## Reference

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## Actinides at the Extremes

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We have been continuously funded by the NNSA Stewardship Science Academic Alliances (SSAA) Program since 2002 to perform fundamental research at the extremes of high pressure, high magnetic fields and ultra-low temperatures in order to reveal the intrinsic physical properties of strategic materials located in the actinide series of the periodic table. Eleven post doctoral researchers, three graduate students and 10 undergraduates have participated in our SSAA research since 2002. One post doctorate researcher, one graduate student, five undergraduate students and two high school students are currently supported by NNSA (see Figure 1).


Figure 1. Some of the post doctorate researchers and students (graduate, undergraduate and high school) who were part of our DOE NNSA collaboration during the past year.

The SSAA Program has enabled us to pursue goals directly related to understanding stockpile stewardship relevant material properties. A strong collaboration has developed with the staff at Los Alamos National Laboratory (LANL) and at Argonne National laboratory (ANL). The frequent lab visits of our students and post doctorate researchers provide ample opportunities to explore NNSA career opportunities.

Two strategic and challenging materials are central to our effort: uranium (U) and cerium (Ce). To aid us, we are exploring complementary materials to push the leading edge of our techniques forward in order to better understand these two elements. High pressure combined with high magnetic fields and low temperatures are used to select and explore the most basic properties that govern macroscopic behavior such as swelling in α–U and the volume collapses found in the plutonium analogue, Ce.

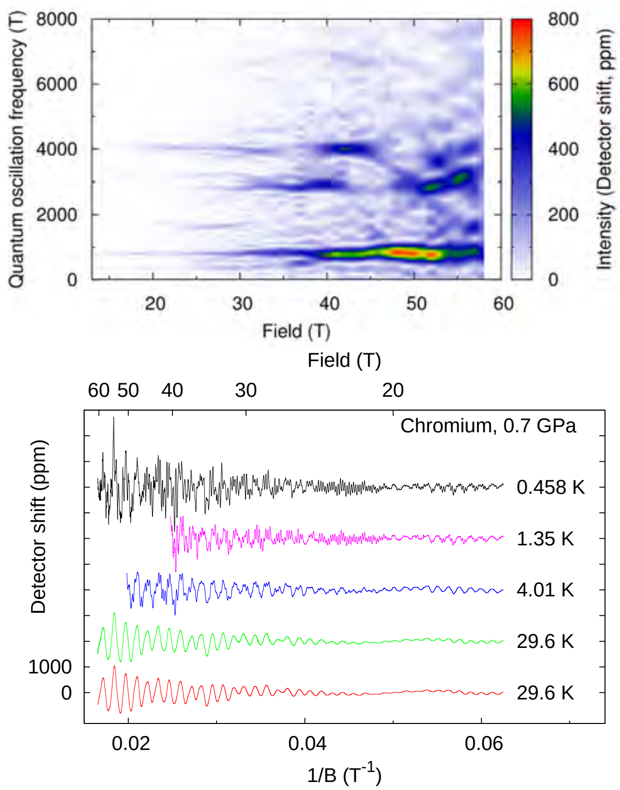


Figure 2. Top - Frequencies of SdH quantum oscillations (a means to probe the mobile electrons that dictate many of material's macroscopic properties) versus applied magnetic field for Cr at 458 mK and 0.7 gigapascal (GPa). Bottom - Raw data (7th order background subtraction) at 0.7 GPa for various temperatures. The 458 mK trace was used to generate the color plot.

Cr is a system that highlights the challenges faced as we proceed with our research on uranium. J. Cooley (LANL MST-16) has instructed our students on how to grow Cr crystals for this project. He has been instrumental in developing sample preparation and annealing protocols to ensure the materials are of the highest quality. The complicated Fermi surface of Cr and existence of a spin-flip transition at low temperatures and high pressures makes it an ideal material to hone student's technical and analytical skill sets. Plastic high pressure cells[1] coupled with a greatly refined resonant tank circuit technique and custom data acquisition and analysis packages allowed us to clearly observe the evolution of the Fermi surface when using the 60 T long pulse magnet at LANL. The experimental conditions were of such high quality that Shubnikov-de Haas (SdH) quantum oscillations were clearly visible in the raw data (see Figure 2).

These techniques and crystal growth enhancements, made possible by our collaboration with NNSA, are being used to study U and Ce, and are being transferred to DOE laboratories for the further study of strategic materials.

### Reference

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# Inelastic X-ray Scattering for High Energy Density Science

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Under the National Laser Users' Facility (NLUF) program, we have collaborated with researchers at Lawrence Livermore National Laboratory (Dr. Siegfried Glenzer and his colleagues) on studies of plasmas using high energy lasers to compress matter and x-ray scattering (inelastic or Thomson scattering) to probe the matter.

Science that is relevant to stockpile stewardship, such as simulations of matter at extreme conditions, relies on very accurate descriptions of plasma physics. It is critical to use experimental platforms that can test models that represent the interactions of radiation with matter as well as the behavior of plasmas at extreme temperatures, pressures, and densities. The results from this research can be used to increase our understanding of physics codes and simulations that are used to expand our physical understanding of how matter behaves under extreme conditions.

The implosion phase of inertial confinement fusion experiments have been predicted to approach high-pressures and densities that can be characterized in a regime of material physics that is extremely hot and dense. Such a regime presents severe challenges to experimental characterization and theoretical modeling. Under such extreme conditions, direct and accurate measurements of physical properties are important in order to test and verify dense plasma modeling along with addressing fundamental physics questions such as the equation of state (EOS) and the structure of the shock-compressed matter.

X-ray Thomson (inelastic) scattering is an excellent *in situ* diagnostic that can be used to fully characterize the properties of dense plasmas. While such scattering has previously been applied to shock-heated matter in proof-of-principle planar geometries, we performed measurements of the electron densities, electron temperatures, and ionization states of spherically compressed multi-shocked CH (polystyrene) capsules through the use of spectrally resolved x-ray Thomson scattering. Laser beams from the OMEGA laser system (45 laser beams with 300 J of energy per beam) were used to compress a CH shell to well above solid density, using coalescing shocks. Separately, a laser-produced high-energy zinc He-α x-ray source (at 9 keV) was used to probe the plasma at a scattering angle of 135 degrees (see Figure 1).

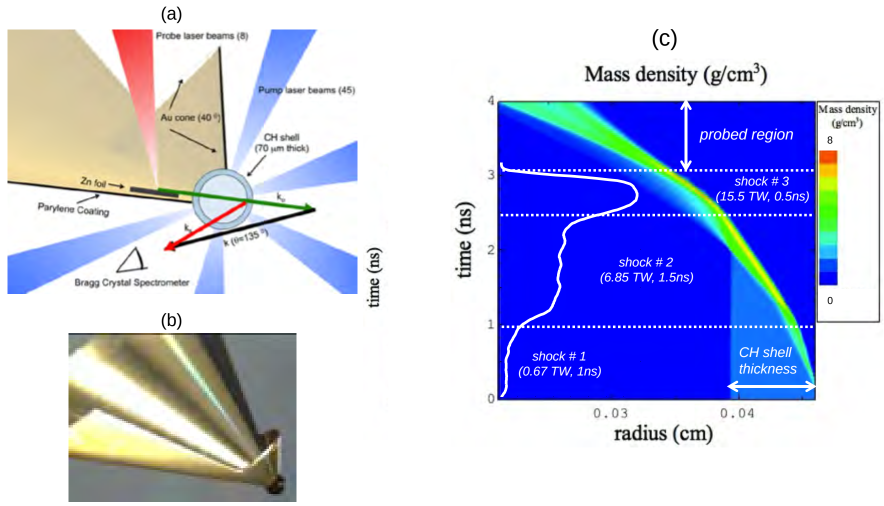


Figure 1. The experimental setup to study spherically convergent coalescing shocks in CH capsules. (a) Schematic diagram of the target geometry, laser beam configuration, and scattering geometry. (b) Photo of CH cone- in-half-shell target. (c) 2D hydrodynamic simulation of the mass density is shown as a function of CH shell radius, and input pulse shape dimensions.

The ability to reach extreme states of hot and dense matter through the use of coalescing shocks enables us to accurately evaluate the EOS of highly non-ideal plasmas and, thus, study how material structure changes at densities and temperatures that have not been previously accessible. The results (see Figure 2) demonstrate the ability to understand the electron temperature, electron density, and ionization state of multi-shock compressed CH capsules using x-ray Thomson scattering techniques. These measurements provide a full characterization of the heating process, enabling a complete description of the time-dependent hydrodynamic evolution of shock-compressed CH, and can be used as a platform to test current EOS models of the material under such extreme conditions.

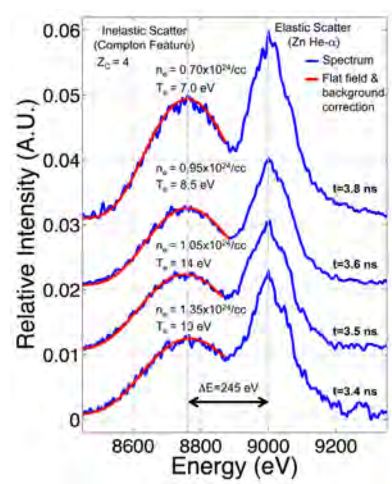


Figure 2. Thomson scattering curve fit analysis. Measured scattered spectra (blue) and best fit (red) to the Compton x-ray scatter features from multi-shocked CH ablators at three times, yielding $n_e$, $T_e$, and Z.

Our experiments under the NLUF program push the limits of what is and is not possible in probing high density plasmas, and help us understand the complex physics at this boundary. This funding has directly contributed to multiple experiments, publications, and collaborations that expand over a number of universities and national laboratories. It has helped to promote novel discoveries that can be applied to the goals that are relevant to the academic and national laboratory communities.

## High-Intensity Laser Interactions with Low-Density Plasmas

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Since 2009, the National Laser Users' Facility (NLUF) program has funded our experiments using the OMEGA EP facility to study low-density plasma interactions with relativistic intensity laser pulses. This support has allowed our experimental team, including graduate student Calvin Zulick, to extend our research from university-scale laser systems, to the larger NNSA National Laboratory facilities. This provides the graduate students with a broader research perspective and links to collaborators at national laboratories.

The hole-boring fast ignition scheme for inertial confinement fusion, where a channel is formed through millimeter-scale low-density plasma to access the dense fuel core, requires knowledge of channeling phenomena through underdense[1] and near-critical density[2] plasmas. Understanding energy transfer from the laser into hot electrons is especially important since the electron heating and motion governs the entire interaction through large electromagnetic fields, channel formation, ion acceleration and x-ray production.

The high-power OMEGA EP laser pulse was focused into an underdense plasma plume where the ponderomotive force of the laser expels plasma electrons to form a channel containing large quasi-static electromagnetic fields. The second orthogonal short-pulse beam on OMEGA EP was utilized to accelerate a proton probe beam, which produced temporally resolved images of the channel fields. Figure 1 shows the channel formation imaged by the proton probe with picosecond resolution from a single 55 J, 1 ps shot. A channel is formed at focus, before the laser breaks up producing several channel filaments along which a modulation is observed.[1] Direct laser acceleration of electrons can occur through the coupling of the channel fields with the laser fields, which can accelerate electrons to many times the ponderomotive energy. Figure 2 shows typical experimental electron spectra, measured using an on-axis magnetic spectrometer, from shots with different laser conditions and

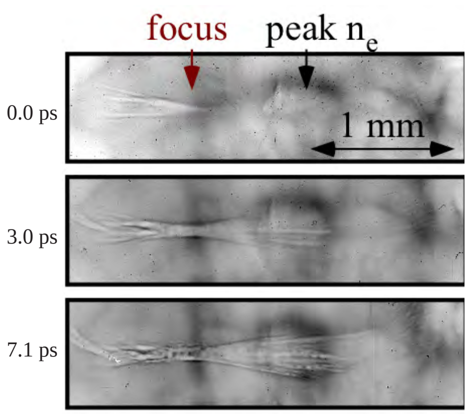


Figure 1. A sequence of proton probe images showing the channel formation by a 1 ps, 55 J laser interaction.

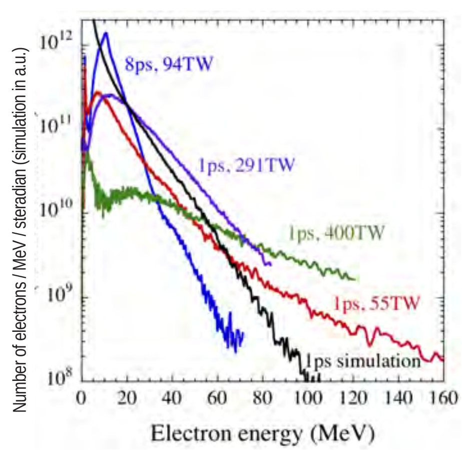


Figure 2. Typical experimental and simulated electron spectra from different laser conditions.

a particle-in-cell simulated electron spectrum, which illustrate the very hot electron temperatures achieved in the underdense interactions. The proton probe images provide evidence for surface wave excitation, which is a likely injection mechanism to supply heated electrons into the center of the channel where the high-intensity laser can further accelerate electrons.[3]

Other phenomena also studied during this shot series were late time channel evolution, ion acceleration, neutron production and near-critical density interactions using very low-density foam targets.[2] The fundamental interaction physics of low-density plasmas are highly complex and non-linear and basic understanding is likely to be relevant to understanding higher density solid targets interactions where a pre-plasma scale length is commonly found.

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# Spectrally-Resolved Imaging of ICF Experiments with the MMI X-ray Imager

University of Nevada, Reno
PI: Roberto C. Mancini, rcman@unr.edu

The research group of Dr. Roberto C. Mancini has been working on x-ray spectroscopy of inertial confinement fusion (ICF) implosion experiments at OMEGA with support from the National Laser Users' Facility (NLUF) program since 2000. The goal of this work has been the diagnosis of time-resolved, space-integrated and space-resolved implosion core conditions, including temperature and density spatial distributions and mixing, and temperature and density conditions and multi-view areal-density maps of the compressed shell confining the core. Currently, two graduate students, Heather Johns and Tirtha Joshi, are working in NLUF research as part of their PhD dissertation projects, and one undergraduate student, Samantha Nasewicz, for her senior thesis work. Over the years, one post doctoral researcher, six graduate students, and two undergraduate students have been supported by the NLUF program. Several former students of the principal investigator (PI) have been hired by national laboratories, including Drs. Peter Hakel (PhD 2001), Manolo Sherrill (PhD 2003), and Leslie Welser-Sherrill (PhD 2006), all by Los Alamos National Laboratory, and Dr. Taisuke Nagayama (PhD 2011) by Sandia National Laboratories.

"The support of the NLUF program has been critical to develop our program on x-ray spectroscopy of ICF implosions through financial support for the students and also for the opportunity to develop a new instrument, i.e., the x-ray multi-monochromatic imager (MMI). We also received access to perform experiments at OMEGA so our program can integrate experiments and observations with theory/modeling and data analysis," said Dr. Mancini.

The MMI instrument was developed by the PI in collaboration with Drs. Jeffrey Koch and Riccardo Tommasini from Lawrence Livermore National Laboratory, first, for recording arrays of spectrally resolved images in indirect-drive ICF experiments and then, for application in direct-drive implosions as well. The instrument combines pinhole-array imaging with the dispersion of a Bragg multi-layer mirror, and the time-resolution provided by a framing camera detector (see Figure 1). Spectrally resolved images can be thought of as "multi-color" images where each one is characteristic of a slightly different color. The data recorded with MMI is space-, time- and spectrally-resolved, rich in information, and it has opened up a new era in the x-ray spectroscopy of ICF implosion experiments, and high energy density plasmas in general. The availability of three identical MMI instruments at OMEGA permits symmetry studies of ICF implosions. As an illustration, Figure 2 shows areal-density surface-plots observed along three quasi-orthogonal lines-of-sight (LOS) extracted from the absorption signature of a Ti tracer in the target. They clearly show the modulations in areal-density observed in each LOS as well as the differences between LOS. These results provide three-dimensional (3D) information about the stability and symmetry of the implosion. This research has also led to a new type of tomography, i.e., polychromatic tomography, where observations taken along a limited number of views are complemented with the information encoded in multiple "colors" or wavelengths in order to reconstruct the 3D spatial structure in the plasma. The development of polychromatic tomography has also motivated a new type of data analysis technique: multi-objective data analysis driven by a Pareto genetic algorithm. The key question addressed by this technique is: *What can be extracted by analyzing simultaneously and self-consistently multiple pieces of data that cannot be extracted by the analysis of each piece of data on an individual basis?* The idea of this analysis method is general and can be applied to spectroscopic as well as other types and combinations of data.

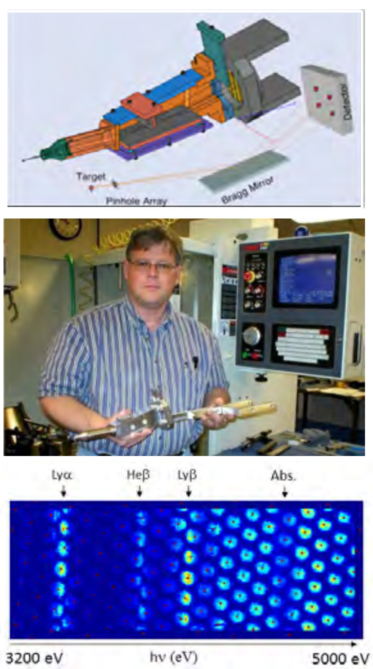



Figure 1. Schematic illustration of the MMI instrument (top) and technician Wade Cline holding one of three identical MMI instruments fabricated at the UNR Physics machine shop (middle). Array of gated spectrally resolved images recorded with MMI in OMEGA shot 49956. Line emissions and absorption due to argon and titanium tracers in the target are visible in the data. Red dots indicate image centers (bottom).

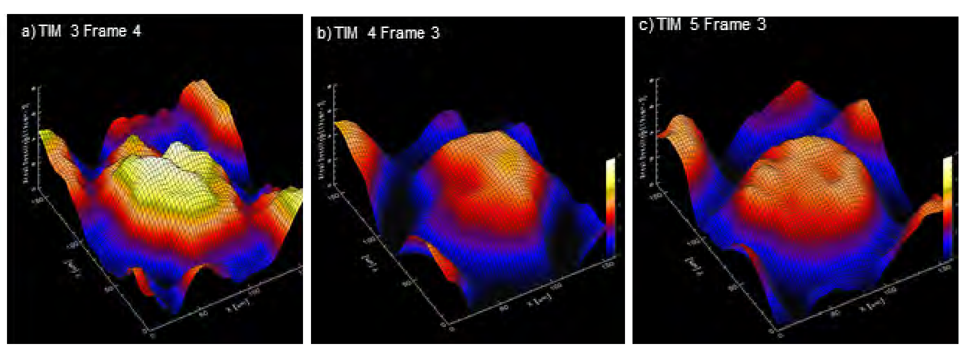



Figure 2. Areal-density surface-plots extracted from the absorption signature of a Ti tracer embedded in the target's shell. The data was recorded in OMEGA shot 49953 with three identical MMI instruments mounted on quasi-orthogonal LOS and for frames approximately simultaneous in time. The x- and y-axis ranges are from 0μm to 160μm, and the z-axis range is from 0 Ti-atoms/cm$^2$ to 8x10$^{19}$ Ti-atoms/cm$^2$, or approximately 45mg/cm$^2$ of plastic areal density. This areal-density is only due to the compressed plastic of the Ti-doped tracer layer.

# Fast Electron Beam Dynamics in High Intensity Laser Matter Interactions for 10-ps Pulse Duration

General Atomics
PIs: R.B. Stephens, rich.stephens@gat.com and M.S. Wei, weims@fusion.gat.com

This National Laser Users' Facility (NLUF) project investigates fast electron beam generation and transport in high-energy (>1 kJ) high-intensity laser/plasma interaction (LPI) over 10-ps pulse duration. This regime is extremely important for development of the fast ignition (FI) approach to high gain inertial fusion energy for which ignition is triggered by fast heating (~10 ps) of a pre-compressed high-density core by fast electrons (1-3 MeV) produced in relativistic LPI. Crucial elements in this process include the following electron source characteristics: photon-electron energy conversion efficiency, fast electron energy spectrum, angular divergence, and emission direction. They depend on the details of a nonlinear LPI process that dynamically evolves with time. Most previous studies have been limited to sub-ps pulses because of limited short-pulse laser beam energies ~100 J). Our investigation took advantage of the high-energy (~1.5 kJ) OMEGA EP facility at the University of Rochester Laboratory for Laser Energetics (LLE) that allows extending such studies to FI-relevant 10-ps pulses. In collaboration with researchers from the University of California, San Diego (UCSD); University of Nevada, Reno; LLE; and Lawrence Livermore National Laboratory, this investigation combines experiments and particle-in-cell (PIC) modeling to facilitate physics understanding and to optimize FI target design for achieving an improved energy coupling for FI. The project supports one UCSD graduate student.

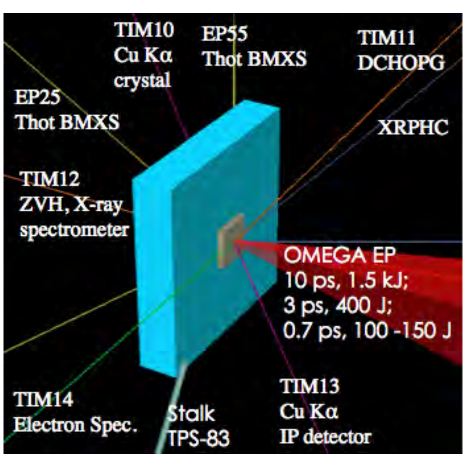



Figure 1. Schematic of the OMEGA EP experimental setup.

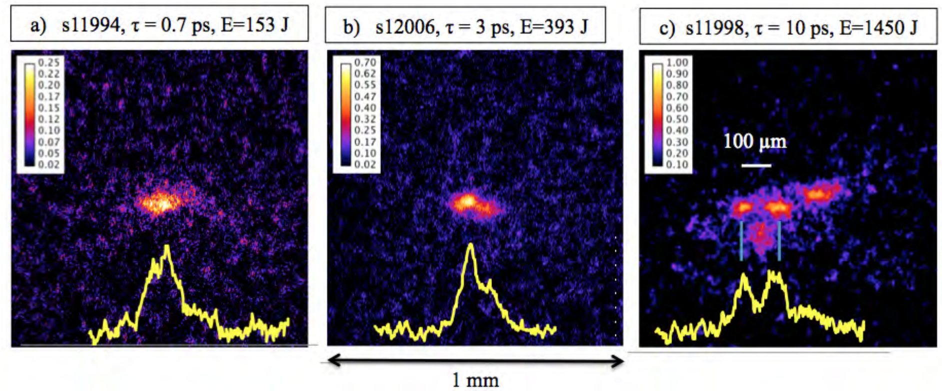



Figure 2. Cu Kα fluorescence images showing fast-electron beam cross-section ~100 μm below the generating point using a laser pulse of (a) 0.7 ps, 153 J, (b) 3 ps 393 J, (c) 10 ps 1450 J pulses in the OMEGA EP experiment. All images are to the same spatial scale. Image is compressed vertically because of the view angle. The yellow lines at the bottom of each image are plots of the pixel intensity along a horizontal line through the points.

Figure 1 shows the experimental setup. The electrons generated at the aluminum (Al) surface of the planar target are detected in a copper (Cu) tracer layer buried ~100 μm below the surface by the fluorescence and high-energy bremsstrahlung emission they generate. A 1-mm thick, 5×5-mm$^2$ carbon back-layer ensured the electrons traversed the Cu layer only once, so that measured signals are directly correlated with the fast electron flux. A Bragg crystal imager shows the electron angular distribution, a calibrated highly ordered pyrolitic graphite x-ray spectrometer measures their absolute number, and two bremsstrahlung spectrometers detect the electron spectrum and laser-to-electron energy conversion. The OMEGA EP backlight beam tightly focused to $R_{80}$~20 μm was adjusted to give the same intensity ($I_{peak}$~$2\times10^{19}$-W/cm$^2$) for pulse lengths of 0.7 ps, 3 ps, and 10 ps with laser pulse energies of ~100-150 J, 400 J, and 1,500 J, and the intrinsic pre-pulse (3-ns long) energies of ~5 mJ, 16 mJ, and 110 mJ, respectively.

The experiment revealed that the LPI evolved over a multiple-ps timescale in a way that strongly modified the resultant fast electron beam. Although the energy conversion efficiency (30% –50%) was found to be similar for all three pulse lengths, the electron spectrum's slope temperature doubled (from 0.7-MeV at 0.7 ps to 1.5 MeV at 10 ps), and the electron beam spatial distribution and emission direction in which the energy was transported changed in a complex manner. Two-dimensional Cu-*Ka* images (see Figure 2) show that the fast electron beam, a single beam in sub-ps LPI with a full width half maximum (FWHM) spot size of ~160 μm, turned, for multi-ps pulses, into several narrow beamlets (each beamlet ~70 μm FWHM) separated from each other by ~45 degrees.

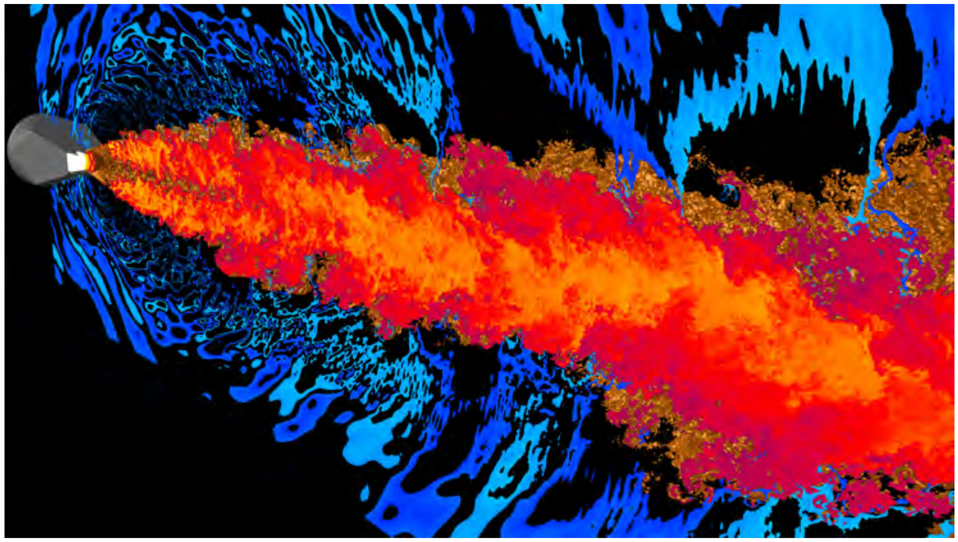
The beam splitting/narrowing was unanticipated. Along with the increase in electron slope-temperature, the splitting/narrowing is suggestive of the development of LPI instabilities over a few ps in the laser-prepulse-produced extended low-density preplasma overlaying the solid dense foil. Preliminary collisional PIC simulations indicate that such a preplasma could filament and self-focus the incoming high intensity laser beam to form a few laser filaments with their propagation angles significantly deviated from the initial propagation direction, resulting in multiple independent, high intensity electron sources. Simulations are underway to add more details to this picture. The PIs want to know the roles played in instabilities growth by pre-existing low-density plasma, and the forces limiting the divergence of these beamlets. A planned NLUF OMEGA EP campaign will use the newly available ultra-high contrast short-pulse beams to examine this LPI evolution in the (initial) absence of an overlying low-density preplasma.

# Predictive Science Academic Alliance Program

## Advanced Simulation and Computing Program

From its earliest days, the Advanced Simulation and Computing (ASC) Program recognized that some program objectives could best be achieved by establishing a strong research portfolio of strategic alliances with leading U.S. academic institutions. ASC's Academic Strategic Alliance Program (ASAP) was formed in 1997 to engage the U.S. academic community in advancing science-based modeling and simulation technologies. In 2008, the Predictive Science Academic Alliance Program (PSAAP) continued this academic engagement by establishing centers at the California Institute of Technology, Stanford University, Purdue University, the University of Michigan, and the University of Texas at Austin, selected through a competition among 34 bidding institutions. These PSAAP Centers focus on the emerging field of predictive science, i.e., the application of verified and validated computational simulations to predict the behavior of complex systems where routine experiments are not feasible. The Centers focus on unclassified applications and science of interest to NNSA and its national laboratories: Lawrence Livermore National Laboratory, Los Alamos National Laboratory and Sandia National Laboratories. The PSAAP Centers develop not only the science and engineering models and software for their large-scale simulations, but also methods associated with the emerging disciplines of verification and validation and uncertainty quantification. The goal of these emerging disciplines is to enable scientists to make precise statements about the degree of confidence they have in their simulation-based predictions. To facilitate the research agendas of the Centers, ASC provides significant cycles on its most powerful, unclassified computing systems.

*These internships introduce students and researchers to the labs and thus increase the likelihood that they will consider the labs for employment or recommend that other students consider the labs for employment. They also expose both national laboratory and Center personnel to research ideas and possible collaborations of mutual interest.*



An image from the jet noise simulation. A new design for an engine nozzle is shown in gray at left. Exhaust temperatures are in red/orange. The sound field is blue/cyan. Chevrons along the nozzle rim enhance turbulent mixing to reduce noise.

*Illustration: Courtesy of the Center for Turbulence Research, Stanford University*

An important component of the program is the requirement that all students supported with PSAAP funds intern at one of the NNSA laboratories at least once for 10 contiguous weeks. Similarly, post doctoral researchers and research staff are required to spend one week annually at one of the NNSA National Laboratories. These internships introduce students and researchers to the labs and thus increase the likelihood that they will consider the labs for employment or recommend that other students consider the labs for employment. They also expose both national laboratory and Center personnel to research ideas and possible collaborations of mutual interest. To date, the Centers have supported 175 students, 18 of which have been hired by the labs.

NNSA's management of PSAAP involves active interactions with the PSAAP Centers. This responsibility rests with the Alliance Strategy Team (AST), which reports to the ASC Executive Committee. A key AST management tool is the yearly, external peer review it organizes for each Center. The reviews focus on the technical progress of the Centers and on providing recommendations to help them meet their goals and milestones. The AST also establishes a Trilab Sponsor Team (TST) for each Center. The TSTs consists of six members, two from each of the three NNSA National Laboratories. The TSTs work with their respective Centers to facilitate interactions with the labs and to provide a forum for discussion on their research directions.

A brief description of the Centers' research follows.

# The Center for the Predictive Modeling and Simulation of High Energy Density Dynamic Response of Materials

California Institute of Technology
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At the California Institute of Technology's (Caltech's) Center, predictive science is demonstrated by means of a concerted and highly integrated experimental, computational, and analytical effort that focuses on an overarching application: hypervelocity normal and oblique impact of metallic projectiles and targets, at velocities up to 10 km/s. Depending on impact velocity and material choices, physics that challenge modeling and simulation include melting, vaporization and plasma formation; solid-solid phase transitions, high-strain-rate deformation and thermomechanical coupling; fracture, fragmentation, spall and ejecta; material instabilities such as shear banding; and hydrodynamic instabilities and mixing. The hypervelocity impact application, in conjunction with a rigorous and novel methodology for model-based uncertainty quantification (UQ), provides the intellectual backbone of the Caltech's Center and its chief organizing principle. In particular, UQ campaigns closely coordinate the experimental, computational, modeling, software development, and verification and validation efforts within an Annual Assessment format.

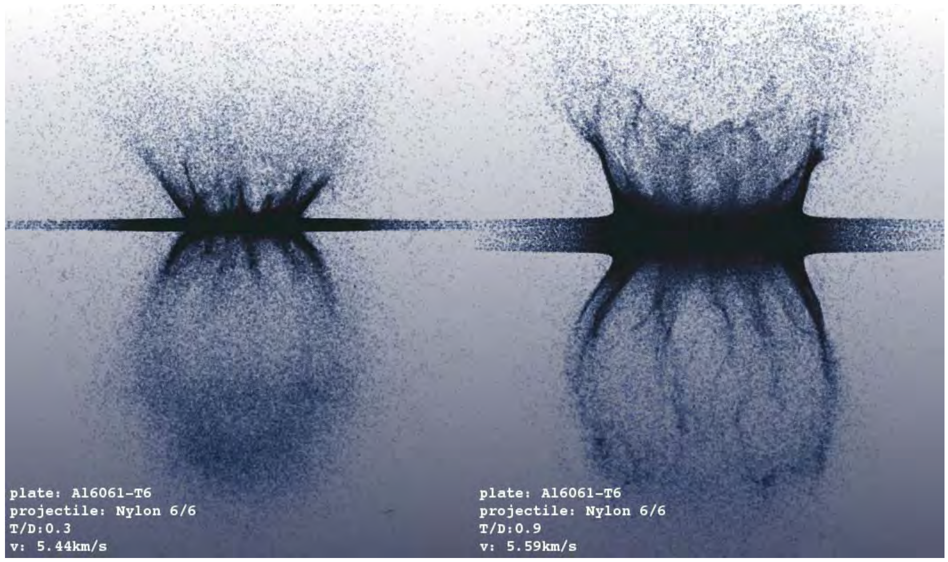


Figure 1. Example of simulation of two hypervelocity-impact experiments performed under the auspices of Caltech's PSAAP Center. A nylon 6/6, 1.67 mm diameter and length, cylindrical projectile strikes Al6061-T6 aluminum plates of two different thicknesses, 0.5 mm (left) and 1.5 mm (right), at 5.44 km/s (left) and 5.59 km/s (right), thereby setting in motion complex physics ranging from an initial impact plasma to fragmentation and debris-cloud formation. The complexity of the material behavior and attendant deformation process render this type of simulation a predictive challenge, and tests the limits of our ability to predict material behavior under extreme conditions. The figures show predicted shadowgraphs showing the structure of the debris cloud in a manner that lends itself to direct full-field, 3D comparisons with experimental data.

This past year has seen the culmination of all of the Caltech Center's efforts and the achievement of its level 1 milestones. With these goals in mind, last year's campaign was designed to push the Center's experimental and predictive capabilities to their fullest. The Center's Small Particle Hypervelocity Impact Range was operated at full capacity with a wide array of diagnostics and metrics, including profilometry, backlighting shadowgraphs, impact-flash spectra, and three-dimensional (3D) debris capture. The resulting extensive data set provided an exacting test of the Center's simulation, material modeling, computational and uncertainty quantification capabilities. Following its usual annual cycle, the center conducted end-to-end Eulerian and Optimal Transportation Meshfree Lagrangian simulations (see Figure 1) for purposes of UQ analysis, leading to a detailed quantification of uncertainties in a number of performance metrics.

The UQ campaign followed the Center's legacy-data optimal UQ protocol, i.e., the experimental campaign preceded the computational campaign and optimal—in the sense of 'tightest'—bounds on probabilities of outcomes were computed that take full account of all the information known about the system, including parameter ranges, validation data, legacy integral data and model errors. The end-to-end simulations were deployed, in a heterogeneous computing mode, on a wide range of platforms at NNSA laboratories, and were managed automatically by the Center's UQ pipeline. The simulations exhibited excellent single-core performance and scalability up to thousands of cores. Both the Lagrangian and Eulerian simulations employed engineering and high-fidelity multiscale models of strength and fracture. A number of key material properties were computed from first principles, including high pressure and temperature viscosities, equations of state, cohesive energies, and others.

As the PSAAP Centers near completion, this is an opportune time to take stock of their accomplishments and ponder their legacy. The challenge handed the Centers at their inception was to advance predictive science through concerted efforts in experimental science, modeling and simulation, and UQ, and to demonstrate those advances in a demanding area of application. The accomplishments of the Centers towards these objectives represent a bold and enduring paradigm shift in predictive science, from hero calculations or experiments to predictions with quantified uncertainties.

## NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems (PRISM)

Purdue University
Center Director: Jayathi Murthy, jmurthy@purdue.edu

During the last few years, there has been a great deal of investment in the development of microelectromechanical systems (MEMS). However, MEMS must satisfy stringent reliability requirements in order to be used in weapons systems. Despite significant effort, MEMS have not thus far been able to meet these criteria, and they experience unexpected failures. Purdue University, in collaboration with the University of Illinois, Urbana-Champaign, University of New Mexico, and Vanderbilt University, has established PRISM to significantly accelerate the development of MEMS technologies through the use of predictive, validated science and petascale computing. The Center seeks to understand, control, and improve the long-term reliability of capacitive contacting radio frequency (RF) MEMS switches by using multiscale, multiphysics simulation, from atoms to micro-devices, to address fundamental failure mechanisms (see Figure 1). Uncertainty quantification (UQ) forms a central unifying theme of the Center. The Center has three specific prediction goals. The first goal is to predict the mean failure lifetime for the case of periodic contact between the membrane and the contact pad of the switch. The second goal is to predict mean failure lifetime for the case of sustained contact, to address dielectric charging. The third goal is to predict critical slopes in the gap-versus-time curves at fixed voltage to capture creep-related failures.

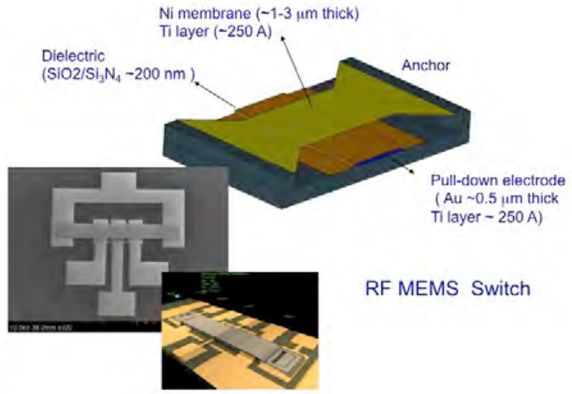


Figure 1. PRISM RF-MEMS Switch.

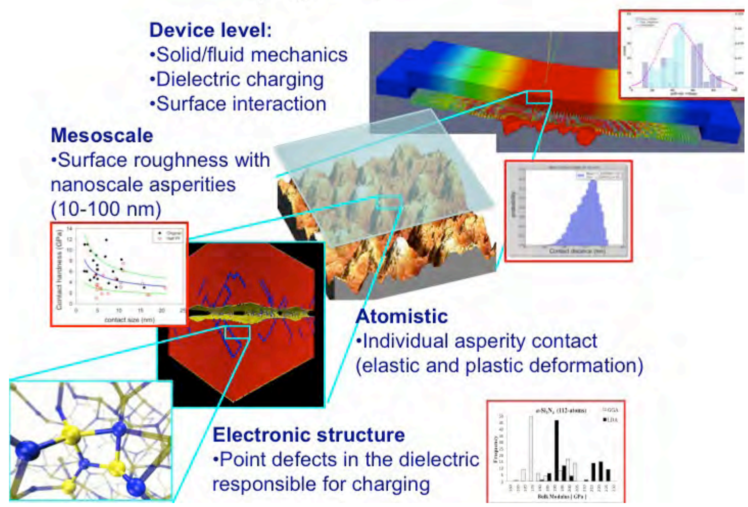


Figure 2. PRISM: multi-physics, multi-scale + UQ.

UQ for these multiscale multiphysics applications poses particular challenges. A singular accomplishment of the Center has been the development and implementation of a unified Bayes network framework for quantifying the combined effects of experimental uncertainty, fabrication variability, and model-form uncertainties. The framework addresses heterogeneity in devices, which include frogleg devices for creep, fixed-fixed membranes and cantilevers. The methodology spans atomistic to device scales and includes model-form uncertainty in atomistic formulations, surface roughness distributions in solid-solid contact, uncertainties in the physics of dielectric charging, and device-level uncertainties in dimensions, physical properties and operating conditions (see Figure 2). Using this framework, probabilistic predictions of contact, creep and charging have been made. This integrated approach has helped identify the most critical models and experiments needed to directly impact prediction accuracy.

Another critical feature of PRISM has been the development of state-of-the-art physical models, numerical methods, and software to address multiscale physics. Of particular note has been the development of a mesoscale contact model incorporating atomistic inputs for surface roughness and elastic constants. Another important contribution has been the development of a multiscale dielectric charging model for amorphous silicon nitride incorporating multiple trap depths, and informed by molecular dynamics and density function theory computations of defect levels and their distributions. Creep models incorporating grain size and orientation effects have also been developed. The coupled ordinate method (COMET) was developed to accelerate convergence and improve scaling of rarefied gas dynamics algorithms.

PRISM has supported a comprehensive graduate and undergraduate educational and research program and a student internship program at the national laboratories. The MEMShub web portal has been developed to disseminate research, software, experimental data and pedagogical materials to the MEMS community.

## The Center for Predictive Simulations of Multi-Physics Flow Phenomena with Application to Integrated Hypersonic Systems

Stanford University
Center Director: Parviz Moin, moin@stanford.edu

The mission of the PSAAP Center at Stanford University is to build and demonstrate computational capabilities for numerical simulations of supersonic combustion engines (scramjet) of hypersonic air-breathing vehicles (see Figure 1). The emphasis of the Center is to evaluate the operability limit of the scramjet as the fuel flow rate is increased. Thermal choking can lead to dramatic loss of performance; simulations can play a critical role in achieving safe operation without over-conservative design.

Faculty from five departments in the School of Engineering at Stanford are involved in the project, together with colleagues from the University of Michigan and State University of New York Stony Brook.

The Center is developing multiphysics computational tools that, combined with an uncertainty quantification (UQ) framework, allow for evaluation of the scramjet performance. The simulation tools benefit from the experience gained in the previous NNSA Center at Stanford; specifically, a common, highly scalable C++/Message Passing Interface infrastructure is deployed to solve the time-dependent compressible, reacting flow equations on three-dimensional (3D) unstructured grids. Both turbulence modeling (RANS) and turbulence resolving simulations are routinely carried out: the former to perform the engineering predictions of the scramjet combustors, the latter to provide data to complement the experimental observations and to guide the assessment of the uncertainties present in the RANS simulations. Discrete adjoint operators are built into the codes and used to provide discretization error estimates for the full system simulations. A closely integrated experimental program provides validation data for the key modeling components, including a novel Monte-Carlo experiment specifically tailored for validation of the UQ framework.

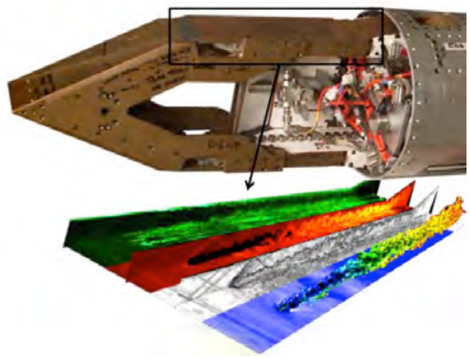

Figure 1. Picture of the HyShot II scramjet engine along with a computed flow field inside the combustor showing the four hydrogen fuel jets and the complex system of shock waves characteristic of supersonic combustion.

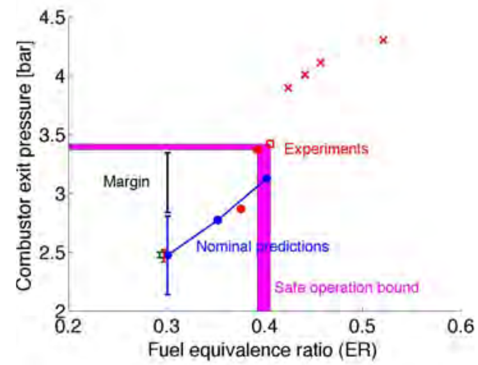


Figure 2. Predictions for HyShot II scramjet operation, both nominal and with uncertainties (error bars at first operating point). Experiments determining the bound of safe operation (solid symbols), and the implied margin between range of predicted operation and range of operability limit.

Quantification of Margins and Uncertainties (QMU) provides the basis for the Center's research and development. In QMU, a metric that characterizes the performance is monitored as a function of the design parameter—the fuel flow rate—within the expected operating scenario. The goal is to determine safe operating conditions by accounting for the uncertainties present while providing a user-specified margin (see Figure 2). Traditionally, UQ methods have been developed that are decoupled from the physics of any specific application. While these methods are useful for some specific uncertainty sources such as the conditions during scramjet operation, a radically different approach is needed for credible UQ of the epistemic (model-form) uncertainty introduced by the turbulence models. One key achievement of the Stanford Center has been the introduction and development of such a UQ approach based on ideas and concepts from hypothesis testing, the physics of turbulence, the geometry of second-rank tensors, and optimization. The uncertainty in the models originates from the hypothesis of alignment between two tensors, the turbulent stress and mean-flow strain rate, used by the vast majority of engineering models. In the approach pursued at Stanford, uncertainty is injected directly into this stress-strain functional relationship by enforcing physical constraints such as realizability. In addition to model uncertainties, we are considering two sources of aleatory uncertainties: variability in the operating scenario and limited knowledge of the reaction rates governing the combustion process. About 30 uncertain parameters are required to describe these two additional sources; the already high computational cost of 3D reacting flow simulations prevents direct sampling, and thus dimension-reduction is a key component of the UQ framework.

A unique component of the Center is the strong collaboration with the Computer Science Department. Software architects and code developers are designing a domain-specific language for mesh-based partial differential equations and demonstrating how a version of the flow solver can map efficiently to a variety of different computer architectures, including multicore and clusters of graphics processing units.

## Center for Radiative Shock Hydrodynamics (CRASH)

University of Michigan
Center Director: R. Paul Drake, rpdrake@umich.edu

The overarching goal of the Center for Radiative Shock Hydrodynamics (CRASH) project is to use scientific methods to assess and to improve the predictive capability of a simulation code, based on a combination of physical and statistical analysis and experimental data. The specific focus of the project is radiative shocks, which develop when shock waves become so fast and hot that the radiation from the shocked matter dominates the energy transport. This, in turn, leads to changes in the shock structure. Radiative shocks are challenging to simulate, as they include phenomena on a range of spatial and temporal scales and involve two types of nonlinear physics: hydrodynamics and radiation transport. To achieve its goal, CRASH focused on a sequence of experiments scheduled for October 2012. These experiments produce a radiative shock in an elliptical tube. The predictions of the results will be based only on experiments using cylindrical tubes combined with computer simulations.

The basic physical system and data from an experiment with a cylindrical tube are shown in Figure 1. Ten (0.35 μm wavelength) laser beams from the OMEGA laser are incident on a 20-μm thick beryllium (Be) disk, at an irradiance of ~ 7 x $10^{14}$ W/cm$^2$ for 1 ns. This shocks the Be and then accelerates the resulting plasma to > 100 km/s. The leading edge of this plasma drives a shock into Xe gas at 1.1 atm pressure with an initial velocity of ~ 200 km/s. This produces the observable structures shown in Figure 1. We have published several papers describing this system and its experimental variability.

Our goal is to predict the primary shock location and metrics measuring wall-shock location (see Figure 1) and shock curvature. The evidence for these predictions comes from sets of simulations using the CRASH code. Briefly, CRASH is a three-dimensional (3D) radiation-hydrodynamic code employing a high-resolution, Godunov-type hydrodynamic solver, flux-limited multigroup diffusion for radiation transport, flux-limited electron heat transport and the necessary related electron physics, a 3D laser-energy deposition package, and tabular treatment of equations of state and opacities. CRASH has adaptive mesh refinement and runs in parallel on massively parallel computers.

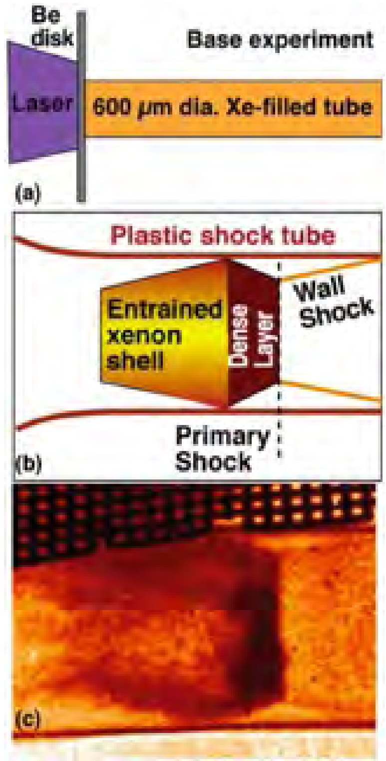


Figure 1. (a) Schematic of a radiative shock experiment. (b) Schematic of features in radiograph. (c) Radiograph.

To formulate the prediction and prediction uncertainty, we combine information from two simulation datasets and data from experiments using cylindrical tubes. The simulation data to integrate into the predictive framework comes from RS12, 128 simulations varying parameters for the 575-μm ID, cylindrical tube, and RS13, 64 simulations varying parameters for the elliptical case (see Figure 2). Because these simulations involve handling large amounts of data, the extraction of the output data from the results is automated. The data extraction routines have been designed to act both on the simulated data and the experimental data, in order to be able to make direct comparisons. This information is combined using the Kennedy-O'Hagan framework utilizing Bayesian Gaussian process emulators. At this writing, we are carrying out this analysis to predict the metrics of interest and their uncertainties for the experiments with elliptical tubes.

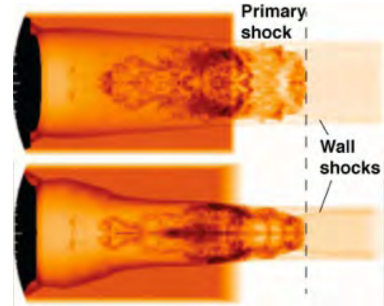


Figure 2. Simulated radiographs from a simulation of the experiment with an elliptical tube, from RS13 at 27 ns. This shock tube has an initial, cylindrical section and a nozzle through which the cross-section changes to an elliptical one. Top-View of major axis. Bottom-View of minor axis.

## The Center for Predictive Engineering and Computational Sciences

University of Texas at Austin
Center Director: Robert Moser, rmoser@ices.utexas.edu

The Center for Predictive Engineering and Computational Sciences (PECOS) is a PSAAP Center within the Institute for Computational Engineering and Sciences at The University of Texas at Austin. The goal of the Center is to develop the next generation of advanced computational methods for predictive simulation of multiscale, multiphysics phenomena, and to apply these methods to the analysis of vehicles reentering the atmosphere.

Simulation of vehicle reentry into the atmosphere is a challenging problem involving many complex physical phenomena such as aerothermochemistry, thermal radiation, turbulence and the response of complex materials to extreme conditions. These arise from the interaction of extremely high temperature gas flows with the vehicle's thermal protection system. An example of a typical simulation for the full system is shown in Figure 1.

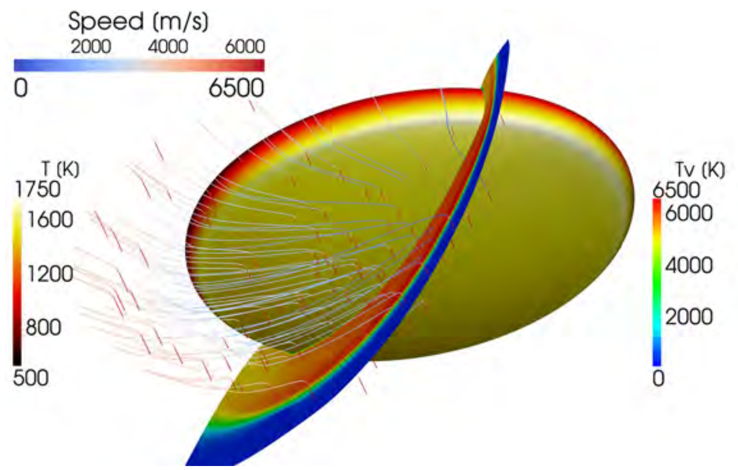


Figure 1. Symmetric capsule at 19.8 degrees angle of attack at Mach 21. Flow conditions are intended to model the peak heating point of an International Space Station entry trajectory. The stream traces are colored by speed while the surface is colored by translational temperature and the flow slice is colored by vibrational temperature. The solution was computed using the FIN-S code developed jointly at the university and NASA Johnson Space Center.

PECOS has recently validated results from their multiphysics hypersonic flow simulator Fully Implicit Navier-Stokes (FIN-S) using the arc-jet experiments used by NASA for high-enthalpy, long-duration material response testing. The NASA arc-jet data corroborated computationally predicted FIN-S heat flux values along a cool catalytic boundary in a high-speed reacting flow. Figure 2 shows a simulation of the arcjet facility at nominal operating conditions.

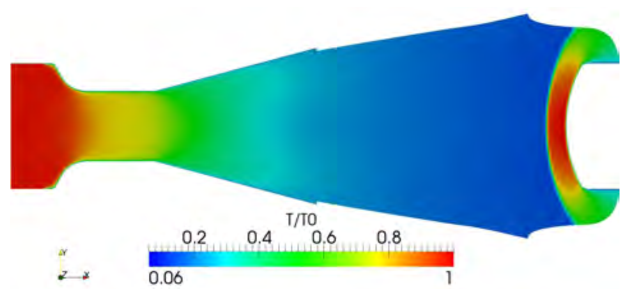


Figure 2. Simulation of NASA Johnson Space Center arcjet facility at nominal operating conditions. The (normalized) temperature field is plotted here. Flow enters the plenum on the left at low speed and high pressure, then accelerates to supersonic speeds through the nozzle and heats the specimen on the right.

Whereas more traditional hypersonic flow codes employ finite volume discretizations and use large numbers of semi-explicit pseudo-time-steps to arrive at converged solutions, the adaptive, implicit stabilized finite element formulations in FIN-S often arrive at steady or quasi-steady flow solutions using an order of magnitude fewer time steps. Finite element and adaptively meshed formulations have been the object of suspicion in the hypersonic flow community regarding their capability to accurately predict surface flux-based quantities of interest. FIN-S is capable of using goal-oriented adaptivity to avoid over-refinement of global mesh features and to reserve mesh resolution for spatial locations which have been predicted by a posteriori error estimators to have the highest contributions to post-processed error in chosen quantities of interest such as the surface peak heat flux. A priori mesh grading is still used to deliver a properly resolved viscous boundary layer around surfaces of interest, but even within the boundary layer, higher fidelity can be subsequently achieved with automatic mesh refinement.

# Unique Opportunities for NNSA Science at the Advanced Photon Source

Carnegie Institution of Washington and Washington State University
PIs: Russell J. Hemley, r.hemley@gl.ciw.edu, Stephen A. Gramsch, s.gramsch@gl.ciw.edu, and Yogendra M. Gupta, ymgupta@wsu.edu

*DOE/NNSA is growing its support of cutting-edge experimental facilities for exploring investigations of materials behavior in extreme conditions at the Advanced Photon Source (APS) at Argonne National Laboratory.*

## The High Pressure Collaborative Access Team: Redefining the State of the Art in High Pressure Research by S. Gramsch and R. Hemley, Carnegie Institution of Washington

The High Pressure Collaborative Access Team (HPCAT) is an integrated facility dedicated to hard x-ray diffraction and spectroscopy of materials under extreme conditions. Operational since 2003, HPCAT (APS Sector 16) is managed by the Carnegie Institution of Washington, and includes partner groups from Carnegie and Lawrence Livermore National Laboratory, along with Stewardship Science Academic Alliances Centers at the University of Nevada, Las Vegas, and Carnegie/DOE Alliance Center. Experimental capabilities are available at HPCAT for fundamental studies in physics, chemistry, materials science, geoscience, and planetary science from ambient pressure to above 300 GPa and temperatures from 4K to 6,000 K. Since user operations began in 2003, there have been over 3,900 person-visits to HPCAT, and over 602 peer-reviewed papers have been published, more than 60% of these representing graduate student and postdoctoral training.

The HPCAT Sector currently consists of four experimental stations, two each on both the insertion device (ID) and bending magnet (BM) beamlines. Station 16-ID-B supports microdiffraction studies with a dual-table arrangement that allows both laser heating and cryostat capabilities. Station 16-ID-D (see Figure 1) supports a variety of x-ray spectroscopies, including emission, inelastic scattering and nuclear resonant techniques. Work in Station 16-BM-B focuses on white beam Laue diffraction and studies involving the use of the Paris-Edinburgh cell. Station 16-BM-D features microdiffraction capabilities in both monochromatic and white beam operational modes.

A large end station on the ID beamline offers room for expansion in the future and was the site of a gas gun experiment in 2009, in which the feasibility of carrying out synchrotron measurements of dynamic compression of materials was demonstrated. A planned upgrade of HPCAT will take advantage of the forthcoming major upgrade of the APS and will bring new capabilities in imaging and dynamics studies of materials in extreme conditions important for NNSA science.

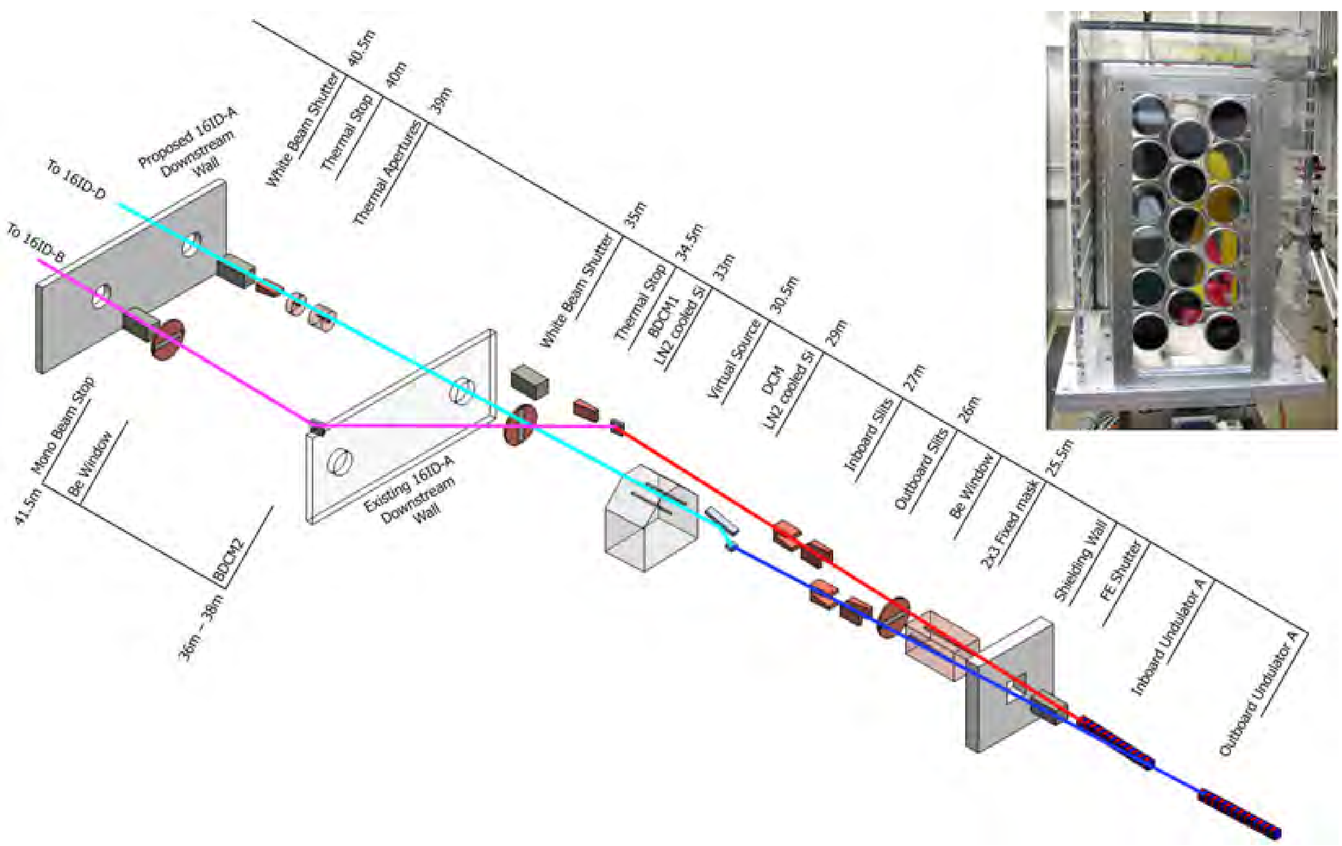


Figure 1. Diagram of the insertion device (ID) beam path at HPCAT. Two undulators in a canted configuration allow independent operation of the microdiffraction and spectroscopy stations. Also shown is the 17-element analyzer for use in x-ray Raman measurements of materials in extreme environments.

## Dynamic Compression Sector at the Advanced Photon Source: A New Paradigm for Understanding Materials at Extreme Conditions

by Y. Gupta, Washington State University

*DOE/NNSA is growing its support of cutting-edge experimental facilities for exploring investigations of materials behavior in extreme conditions at the Advanced Photon Source (APS) at Argonne National Laboratory.*

Understanding the real-time, atomistic-level response of materials under dynamic conditions is central to the Stockpile Stewardship Program, to fundamental science frontiers in numerous fields, and to advanced technology. To address this key scientific need, the DOE/NNSA is establishing a first-of-a-kind user facility at the APS. Washington State University is partnering with the APS to establish the Dynamic Compression Sector (DCS), an experimental capability dedicated to time-resolved (~ns resolution), multi-scale measurements in dynamically compressed materials.

DCS will couple a variety of dynamic compression platforms to a state-of-the-art synchrotron beamline, with tunable x-ray energies and time-structures (ns-separated pulses), to obtain x-ray diffraction and imaging measurements simultaneously with continuum measurements to observe time-dependent changes in materials subjected to a broad range of peak stresses (~ 5 GPa to well above 100 GPa) and time-durations (~ 10 ns to ~ 1 μs). DCS will be used to probe condensed matter phenomena, such as structural transformations, inelastic deformation and fracture, and chemical reactions "on-the-fly" or as they occur. Figure 1 shows the layout of the experimental stations in Sector 35. Three stations will be dedicated to dynamic compression platforms and one station will be reserved for non-single event or longer duration time-resolved experiments. Commissioning and first experiments are planned for spring of 2014. This NNSA-sponsored user facility represents a new paradigm that integrates the expertise/interests of NNSA laboratories and academic institutions to undertake scientific discovery challenges and to train the next generation of scientists. The combination of DCS and HPCAT at the APS will provide a unique scientific environment for increasing the understanding of material behavior at extreme conditions.

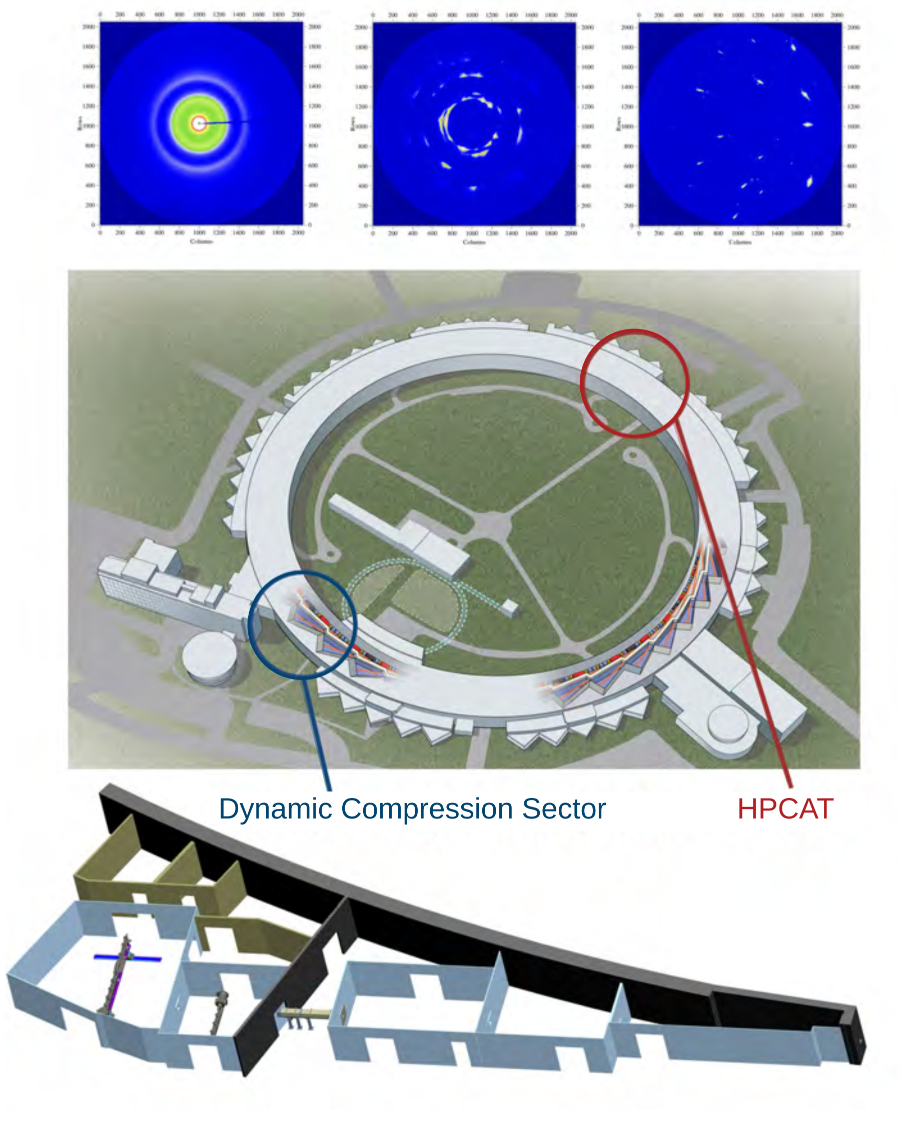


Figure 1. Top - Single-pulse charge coupled device images demonstrating the use of a 100 ps x-ray pulse to obtain diffraction data on a variety of materials. Consecutive images will be used to assemble a movie. Middle - View of the APS. Bottom - Three-dimensional layout of the DCS Sector.

## Brett Manning

brettman@physics.rutgers.edu

### Degree in Progress

PhD candidate, Nuclear Physics, Rutgers University; Advisor: Dr. Jolie Cizewski

### SSAA Program Years

2009 - present

### Research Topic

Single-Neutron States in Neutron-Rich Sn Isotopes

### Research Responsibilities

My responsibilities span the entire spectrum involving transfer reactions. One day, I could be making plastic targets for an experiment, and the next I could be building detectors. I really like working with Jolie Cizewski at Rutgers because her group covers every aspect of an experiment, from the electronics setup to the final analysis in conjunction with a theorist.

### Benefits of the SSAA Program

The SSAA Program has provided the opportunity to travel all over the country for experiments and conferences. This time spent traveling has opened my eyes to the possibilities in the field. I have been able to speak in front of many leaders in the field, and this exposure is invaluable when applying for future positions. Furthermore, the time spent at other facilities has broadened my skill set and experience with nuclear physics.

### What Surprised You About the SSAA Program

I think I have been most surprised by the diversity in the program. I fully expected the students to come from several institutions and all be experimental nuclear physicists with highly applied projects. It turns out this was not even close to being true. The students come from all over, and offer varying skill sets.

### Message to Students Considering the SSAA Program

Joining the program will provide an immense amount of career development. It is easy to float through graduate school without understanding the broader context of your work; but you will not leave this program without realizing how your research ties in with the whole nuclear community.

### SSAA Program Influence on Choice of Research Area and University

I was initially considering other branches of physics, but my current adviser showed me all of the opportunities I would have working with her and being a part of the stewardship program. It should come as no surprise that the money available for travel was highly attractive. I ultimately chose to work with Dr. Cizewski at Rutgers because I knew she could put me in position to benefit from this program. Many other students are forced to teach deep into their graduate careers, and have little time to consider professional development and post doctorate opportunities.

### SSAA Program Collaboration Opportunities

It is amazing how many people I have been able to work with due to the program. Our group often runs experiments at Los Alamos National Laboratory and other prominent labs. While at these labs, we work side-by-side with the staff scientists—an invaluable experience.

## Christine Krauland

krauland@umich.edu

### Degree in Progress

PhD candidate, Applied Physics, University of Michigan; Advisor: Dr. R. Paul Drake

### SSAA Program Years

2004 - 2007 (undergraduate)
2007 - present (PhD)

### Research Topic

Our group primarily focuses on laser plasma experiments performed under high energy density conditions that allow us to investigate scaled astrophysical systems. My thesis work has been centered on a novel experiment that explores the contribution of radiative shock waves to the evolving dynamics of binary star-accretion disk systems in which they reside. More specifically, this experiment creates a supersonic plasma flow in vacuum, which becomes shocked and strongly radiates as it cools.

### Research Responsibilities

As a graduate student under Paul Drake, I have the unique opportunity to be the primary principal investigator on all experiments that are tied to my thesis project. Because we use the Laboratory for Laser Energetics (LLE) in Rochester, New York for our research, this requires me to interface with the full range of people from LLE administrative personnel to the laser technicians to diagnostic scientists and engineers. As I have full design responsibility, I also work with machinists and staff at the University of Michigan to oversee the build of our experimental targets. Finally, I work with, analyze, and publish the data from each of these campaigns.

### SSAA Program Influence on Choice of Research Area and University

The SSAA Program is truly the reason I chose the graduate program that I did. As an undergraduate at the University of Michigan, I found Dr. Drake's lab as a sophomore and was hired to do small research projects within the lab. Over the next three years, not only did I find a love of our research field, but more so the ability and opportunities that the SSAA Program allow a student to cultivate.

### Message to Students Considering the SSAA Program

If I could communicate only one piece of information to new graduate students, it would be the amazing opportunity to work with numerous leading scientists. The SSAA Program gave me the chance to present my work at many symposiums, including its annual review, which bore many discussions, collaborations, and overall, much professional exposure.

## Jacob A. McFarland

jacob.a.mcfarland@gmail.com

### Degree in Progress

PhD candidate, Mechanical Engineering, Texas A&M University (TAMU); Advisor: Dr. Devesh Ranjan

### SSAA Program Years

2010 - present

### Research Topic

Shock and Buoyancy Driven Instabilities

### Research Responsibilities

I designed and built the shock tube facility and assisted with the design and construction of a multi-layer Rayleigh-Taylor facility at TAMU. I have mostly been involved with the experiments on the shock tube facility. My role has been to design and perform experiments on shock-interaction with an inclined gaseous interface. I have been responsible for the design and construction of the facility, running simulations of the experiments and publishing results in journals. As part of the construction of the facility, I had the opportunity to do a lot of machining, welding, and fabricating. I also have been able to lead a team of three fellow graduate students and three to four undergraduate students.

### Benefits of the SSAA Program

The SSAA has helped me tremendously, by giving me the opportunity to work with the research group at TAMU and the NNSA labs, and travel to international conferences. As part of my research, I have been able to spend time at Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory (LLNL). I worked at LLNL as part of the high energy density physics summer student program for two summers. This allowed me to learn and use advanced hydrodynamics computer codes, and work with some of the top researchers in my field. I have also been fortunate to have the ability to travel to the International Workshops on the Physics of Compressible Turbulent Mixing conference (London) and the Turbulent Mixing and Beyond conference (Trieste, Italy).

### What Surprised You About the SSAA Program

The amount of cooperation between the NNSA labs and academia. I have worked with researchers at LANL and LLNL, and used their codes to simulate my research while providing them with experimental data and getting their feedback/advice.

### SSAA Program Collaboration Opportunities

Without this program, I may not have been able to develop the good relationship I have with researchers at LANL and LLNL. I have met many researchers from around the world at the conferences I have traveled to and been able to stay in touch with many of them and learn more about their research. The regular feedback from these people has significantly improved the quality of my research.

## Michael Weller

mweller@unr.edu

### Degree in Progress

PhD candidate, Physics, University of Nevada, Reno; Advisor: Dr. Alla Safronova

### SSAA Program Years

2007 - present

### Research Topic

Experimental and Theoretical Studies of Complex Silver and Molybdenum Wire Arrays

### Research Responsibilities

My responsibilities have changed and grown throughout my graduate school career as my knowledge and experience have increased. For now, I predominately work as a theoretician; however, we have experimental campaigns approximately twice a year, lasting from 3 to 5 weeks each, during which I act as an experimentalist. As far as the theoretical part goes, I am responsible for improving and maintaining our breadth of theoretical models, training new students with the theoretical models, and using the models to glean new and exciting research. For example, our main workhorse is our non-LTE kinetic (non-local thermodynamic equilibrium) model which is capable of producing synthetic spectra, which we then compare to experimental spectra to attain approximate plasma conditions, such as electron temperature and density. For the last five years, I have been presenting my work at conferences, while also writing papers for peer reviewed journals (two in the last year). As far as the experimental part goes, I am responsible for all optical diagnostics and data obtained, which includes operating a laser for shadowgraphy probing. Recently I have implemented a new time-integrated hard x-ray spectrometer capable of viewing wavelengths between 1 and 4 Å, depending on the configuration, which was utilized to produce our first ever results of the time evolution of L-shell Ag plasmas. The past three years I have proposed and completed experiments on the Zebra generator at the University of Nevada, Reno, producing exciting results which will go into my dissertation.

### Benefits of the SSAA Program

The correct question should be *How have you not benefitted?* The support from the SSAA Program has completely jump-started my professional physics career, and that alone is enough for me to be truly thankful for the rest of my life. It has also provided me with the opportunity for collaborative work with distinguished scientists such as Dr. Apruzese from the Naval Research Laboratory, Dr. Coverdale from Sandia National Laboratories, and Dr. Beiersdorfer from Lawrence Livermore National Laboratory, to name a few.

## Lisa Mauger

Lmauger@caltech.edu

### Degree in Progress

PhD candidate, Applied Physics, California Institute of Technology; Advisor: Professor Brent Fultz

### SSAA Program Years

2009 - present

### Research Topic

Thermodynamics of Fe-alloys at Elevated Pressures and Temperatures

### Research Responsibilities

My doctorial research focuses on experimental studies of the thermodynamics of Fe-alloys at elevated pressures and temperatures. This work utilizes nuclear resonant x-ray techniques to probe the dynamics of atoms and electrons in alloys as a function of composition, temperature and pressure. Many of my experiments rely on DOE National Laboratory user facilities instruments, where intensely focused x-ray beams are available to probe the small sample volumes permitted in high pressure diamond anvil cells. My research responsibilities include designing experiments, writing proposals, synthesizing samples, developing sample environments, conducting synchrotron experiments, and writing peer-reviewed articles. Since both high pressure techniques and many synchrotron spectroscopy techniques are still actively developing, my experiments require close collaboration with staff at DOE facilities like the Advanced Photon Source.

### Benefits of the SSAA Program

My research on materials under extreme conditions has been supported by the Carnegie/DOE Alliance Center (CDAC) for more than four years now. I have benefitted from both the equipment and expertise of the research scientists at the Carnegie Institution of Washington's Geophysical Laboratory, who are always eager to collaborate. The CDAC student travel support has permitted me to undertake a wide range of experiments at DOE user facilities, developing expertise and collaborations beyond the laboratories of my home institution. I have also benefitted from attending the annual SSAA symposia. These meetings have provided me with a glimpse of the wide range of fundamental research being conducted in support of stockpile stewardship, while demonstrating the complementary nature of this diverse body of work. The SSAA symposia have given me the opportunity to connect with scientists in a wide range of fields, fostering communication and collaboration. I have developed a better understanding of the research programs underway within the NNSA National Laboratories, and the opportunities available within them. The annual SSAA symposium and the CDAC partner workshops have provided me with a network of peers from different institutions with complementary research interests. This network fuels creative collaboration and development, while fostering a sense of community that facilitates greater cooperation at the national user facilities and national scientific meetings.

## William Moore

wmoore@mines.edu

### Degree in Progress

PhD candidate, Nuclear Engineering, Colorado School of Mines; Advisor: Dr. Uwe Greife

### SSAA Program Years

2010 - present

### Research Topic

Instrumentation development for a double arm fission spectrometer to produce experimental data that can be used to supplement and verify advances in theoretical fission models

### Research Responsibilities

My research responsibilities start with the design and construction of the components of my detector, including gas-filled ionization chambers for energy measurement and electrostatic mirrors for manipulating electron trajectories for time of flight measurements in conjunction with microchannel plate detectors. I have been integrating an in-house built waveform digitizer for data collection and have been working on developing algorithms to minimize noise to improve resolution. Other research responsibilities include design and construction of a vacuum chamber for the production of double-sided fission sources to be used for dual arm coincidence measurements.

### SSAA Program Influence on Choice of Research Area and University

I have always been fascinated with nuclear fission because it is a highly complex process with many unanswered questions, even though it has been more than 70 years since its discovery. Although the SSAA Program did not directly draw me to my choice of research, it has provided me with the opportunity to conduct my research on the topic I am most interested in.

### SSAA Program Collaboration Opportunities

The SSAA Program provided me with the funding to support my research which has allowed the Colorado School of Mines to be a part of the Spectrometer for Ion Detection Fission in Fission Research (SPIDER) collaboration, which is led by Fredrik Tovesson at Los Alamos National Laboratory.

## Katie Brown

Los Alamos National Laboratory
kebrown@lanl.gov


**Degree**
PhD, Chemistry, 2012

**SSAA Program Years**
2007 - 2012

**Fellowship**
Agnew National Security Postdoctoral Fellow

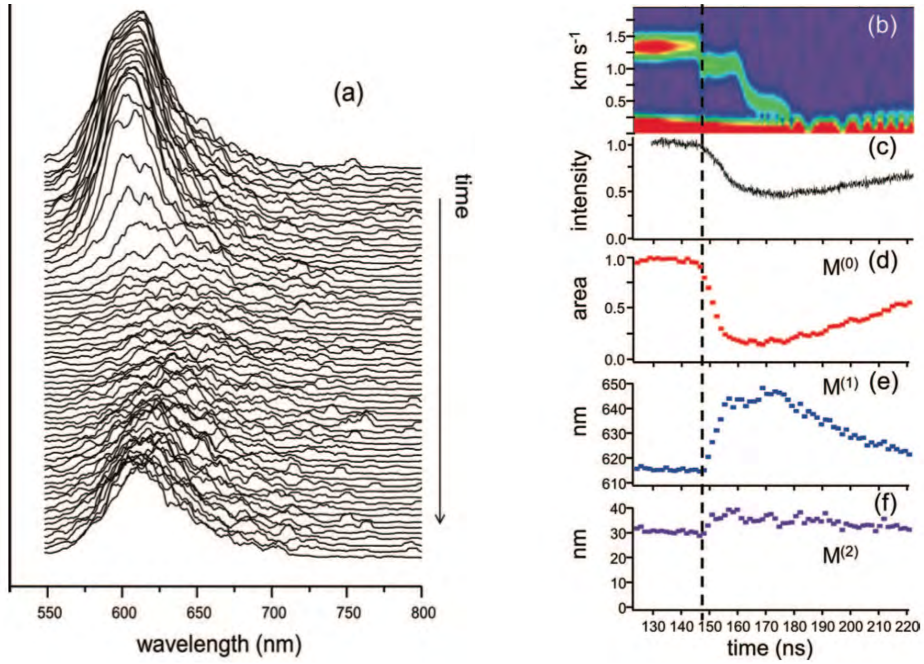


Figure 1. Time-dependent emission from Rhodamine 640 dye in PMMA pumped by a quasi-continuous 527 nm laser, subjected to a 1.3 km $s^{-1}$ impact with a 50 $\mu$m Al foil that produced 4.8 GPa shock pressure. (a) Streak record. The sudden intensity drop is caused by shock redshift of the absorption away from exciting laser line. (b) PDV velocity history. The impact time is denoted by the dashed vertical line. (c) PMT measurement of wavelength-integrated intensity change. (d) Spectral moment 0 of the streak camera data, denoting instantaneous integrated intensity. (e) Spectral moment 1 denoting instantaneous averaged wavelength. (f) Spectral moment 2 denoting instantaneous spectral width.

I was funded by the Stewardship Science Academic Alliances (SSAA) Program through the Carnegie/DOE Alliance Center (CDAC) to study materials under static and shock compression throughout my graduate career in the chemistry department at the University of Illinois at Urbana-Champaign with Dana Dlott. After I joined the group, Dr. Dlott handed me a binder from the previous CDAC review and asked if I wanted to be a part of it. High-pressure research hadn't been anything I'd thought about before graduate school, but it sounded like something I wanted to do, and being part of CDAC was a great opportunity.

My first project in the group was combining surface-enhanced Raman scattering spectroscopy with diamond anvil cell technology to obtain the first known spectra of molecular monolayers under high pressure (J. Phys. Chem. C, 113, 5751, 2009). The remainder of my PhD work involved developing a technique to simultaneously monitor the global and local environments of inhomogeneous materials shocked with laser-driven flyer plates. I used a Rhodamine dye embedded in poly(methyl) methacrylate (PMMA) as a model system. Fluorescence spectroscopy from the embedded Rhodamine dye probes was used to characterize the local environments of the polymer chains, and photon doppler velocimetry (PDV) interferometry was used to measure shocked particle velocities that gave information about the global environments of the microns-thick polymer (Rev. Sci. Instrum., 83, 103901, 2012 and J. Appl. Phys., 112, 103508, 2012). I earned my PhD in 2012 and am now a postdoctoral fellow at Los Alamos National Laboratory (LANL).

Through the CDAC program, I attended several meetings and conferences I would not have otherwise, including four SSAA symposia and two CDAC reviews and workshops. I not only was exposed to other research of materials under extreme conditions, but also to the other branches of stewardship science. Being able to present my research at these meetings was invaluable. It gave me a chance to practice communicating my work and I got a lot of input from knowledgeable people. Most importantly, these meetings were great places to network! I got to meet other graduate students in my field, people with whom I could discuss research problems and genuinely looked forward to seeing every year, and I made amazing professional contacts who are a big part of why I am at LANL. There were often several scientists from the NNSA laboratories who wanted to talk about what their labs were like, pointed me to potential future principal investigators, and encouraged me to stay in the stewardship sciences.

I loved the research I did in graduate school. I decided that I wanted to stay in the field, both because I found the science to be stimulating and interesting, and for the sense of purpose that came with doing research with implications in national security. So far as I could tell, the best place to do the science that I wanted to do was at an NNSA laboratory. I interviewed at LANL and was awarded an Agnew National Security Postdoctoral Fellowship. I started at LANL in September 2012 in the Shock and Detonation Physics group and I am working toward using coherent anti-Stokes Raman scattering (CARS) and CARS imaging to identify the chemical and spatial evolution of reactions taking place in shocked inhomogeneous energetic materials.

I am so excited to be working at LANL in the field of shock dynamics! I'm grateful to the CDAC and SSAA programs for their support during graduate school, and for all the opportunities they gave me to present my work and make connections with professionals in the stewardship sciences.

# SSAA Collaborations in Material Damage Under Extreme Conditions

Authors: Sheng-Nian Luo, LANL; Pedro Peralta, ASU; and Eric Brown, LANL (en_brown@lanl.gov)

Grain boundaries (GBs) play an important role in deformation and spall damage nucleation in shocked metals, a challenging subject relevant to NNSA missions. Scientists at Los Alamos National Laboratory (LANL), i.e., Dr. S.N. Luo and coworkers, and Arizona State University (ASU), i.e., Professor P. Peralta's group, have conducted flyer plate impact experiments, as well as molecular dynamics (MD) and continuum-mechanics simulations, to elucidate the underlying mechanisms and develop practical models. The combined LANL and ASU expertise and resources, in particular the electron microscopy capabilities at ASU, and two-way intellectual inspirations, allow us to tackle this problem efficiently. Without the support of the SSAA Program, productive collaboration between ASU and LANL would be impossible. We have also trained undergraduate and graduate students with valuable hands-on experiences in materials under extreme conditions, who now have the skills to contribute to NNSA missions in the future.

MD simulations of copper bicrystals have been used to correlate deformation and spallation to GB crystallography, particularly coherent twin boundaries (CTBs), and asymmetric or symmetric incoherent twin boundaries (SITBs), which are often formed during processing.[1,2] GB plasticity can be triggered at SITBs by shock, but with more resistance at CTBs.[1] Slip of full and partial dislocations can lead to a high mobility of the SITB, which encourages spall damage nucleation at GB-initiated shear planes rather than at the SITB itself during the release-tension process. In contrast, CTB's low mobility preserves the interface, which becomes the primary nucleation site. The plasticity generated around a SITB is from dislocation movement from the boundary itself, resulting in spallation adjacent to it (see Figures 1a and b). At larger length scales, it might be impossible to discern whether damage nucleates at GB or next to it; however, recent work by Brown et al.[3] suggests that a phenomenon similar to that described above can occur at length scales of the order of the grain size. They compared three-dimensional (3D) experimental observations of damage localization in large grained samples with 3D finite element simulations using a modified Gurson-Tvergaard-Needleman (GTN) damage model combined with crystal plasticity. The results show that for GBs between grains with significant mismatches in plastic behavior, as measured by their Taylor factors, large plastic strain concentrations can be present in the GB affected zone (GBAZ), leading to damage localization (see Figures 1c and d). The agreement between modeling and experimental results (see Figure 1e), where damage can be seen concentrated to the right of the GB, suggests that damage can localize in GBAZ rather than at the GB itself, although the damage should still be considered intergranular. Our work highlights the role of GBAZ in certain "apparent transgranular damage." Furthermore, both strain concentrations and GB strength need to be considered to understand the role of GB on damage nucleation.

*We have also trained undergraduate and graduate students with valuable hands-on experiences in materials under extreme conditions, who now have the skills to contribute to NNSA missions in the future.*

## References

[1]W.Z. Han et al., *Deformation and Spallation of Shocked Cu Bicrystals with Σ3 Coherent and Symmetric Incoherent Twin Boundaries*, Phys. Rev. B 85, 024107, 2012.

[2]S.N. Luo et al., *Shock Wave Loading and Spallation of Copper Bicrystals with Asymmetric Σ3<110> Tilt Grain Boundaries*, J. App. Phys. 108, 093526, 2010.

[3]A. Brown et al., *3-D Characteristics of Local Microstructural Weak Links for Spall Damage in FCC Metals: Geometric and Crystallographic Effects*, Int. J. Plasticity, submitted 2012.

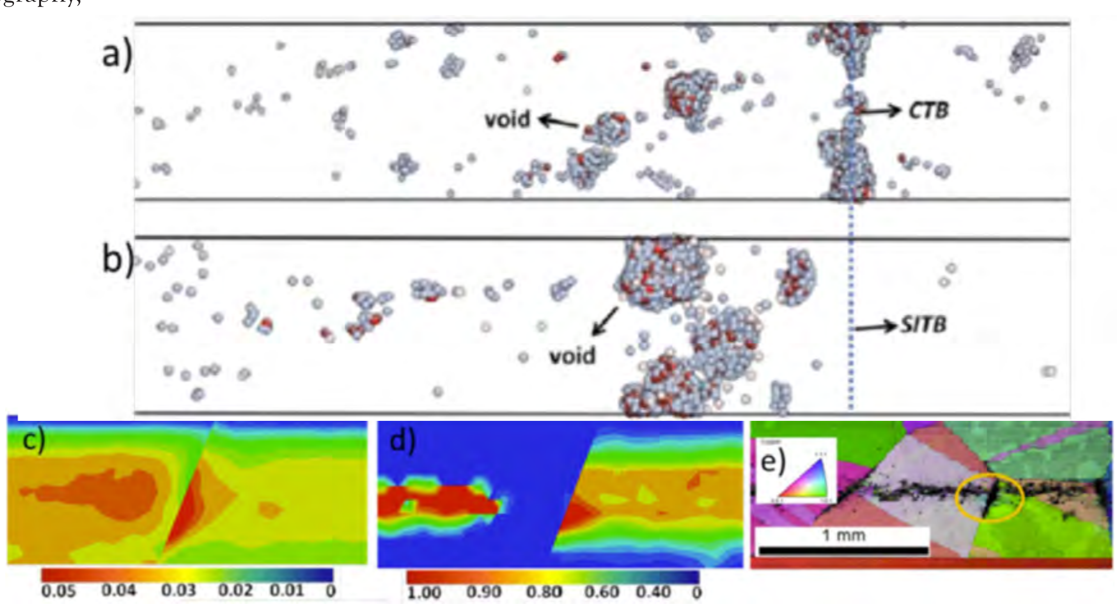


Figure 1. MD simulations showing void nucleation concentration a) at the CTB or b) away from the SITB.[1,2] c) Equivalent plastic strain and d) void volume fraction from modified GTN simulations, compared to e) electron-backscatter-diffraction scan of corresponding damage site.[3]

## SSAA Collaborations in Nuclear Science

Authors: J.T. Burke (burke26@llnl.gov), J.E. Escher, N. Schunck, and N.D. Scielzo

The Stewardship Science Academic Alliances (SSAA) Program has had a tremendous impact on the low-energy nuclear science program at Lawrence Livermore National Laboratory (LLNL). Numerous young researchers, some of whom have been hired at national laboratories, have been trained through collaborations with U.S. institutions: Texas A&M University and its Cyclotron Institute, Rutgers University, the University of Richmond, Ohio University, the Triangle Universities Nuclear Laboratory at North Carolina State University, and the University of Tennessee, as well as groups from the United Kingdom, France, Japan, and Canada. A small group of the over 65 active scientists, postdoctoral researchers, graduate students, and undergraduate students involved in the research program with LLNL is shown in Figure 1.

The activities of the LLNL-related collaborations address important basic science questions such as *How are the elements produced?* and *How do nuclei interact in very neutron-rich environments?* The SSAA Program has created outstanding opportunities for research in a subject area that is both very attractive to students and relevant to the NNSA mission.

The precise determination of nuclear cross sections is crucial for both NNSA programs and for answering the aforementioned questions. Many reactions involve short-lived radioactive nuclei that are difficult or impossible to make into targets (see Figure 2). At LLNL, we measure cross sections of short-lived nuclei, directly and indirectly, and develop predictive theories.

A major research focus has been the development of the surrogate reaction technique,[1] to determine cross sections indirectly via a combination of experiment and theory with the STARLiTe detector array at the Texas A&M Cyclotron Institute. The STARLiTe Collaboration has already determined five new cross sections.

Cross section calculations require reliable nuclear structure data as input. We use multiple techniques, including gamma ray spectroscopy, to determine the structure of nuclei, determine half-lives of nuclear states, and study the density of excited states in nuclei.

Nuclear theory enables us to describe the surrogate reaction technique and other indirect methods, and it facilitates extending their applicability. A predictive theory of the highly complex fission process is an important long-term goal of clear relevance to NNSA that requires a tremendous amount of high-performance computing. Our theory activities have significantly benefited from leverage by other DOE-sponsored research efforts.

*The SSAA Program has created outstanding opportunities for research in a subject area that is both very attractive to students and relevant to the NNSA mission.*

Our partnership with the SSAA Program has directly enhanced the research of LLNL scientists, as shown by collaborative publications (more than 50 in the past 6 years), in peer-reviewed journals, and presentations at national and international conferences.

### Reference

[1]J.E. Escher et al., Reviews of Modern Physics 84, 054619, 2012.

Figure 1. A subset of the STARLiTE Collaboration at the Texas A&M University (TAMU) Cyclotron Institute. Back row, left to right: Brett Manning (Rutgers University), Tim Ross, Richard Hughes, Professor Cornelius Beausang (Richmond), Peter Humby (Yale), Callum Shand (Surrey), William Peters, Andrew Ratkiewicz, Jason Burke (LLNL) and Matt McCleskey (TAMU). Front row, left to right: Erin Good, Kristen Gell (Richmond), Samantha Rice (Rutgers), Professor Roby Austin (St. Mary's), and Professor Jolie Cizewski (Rutgers).

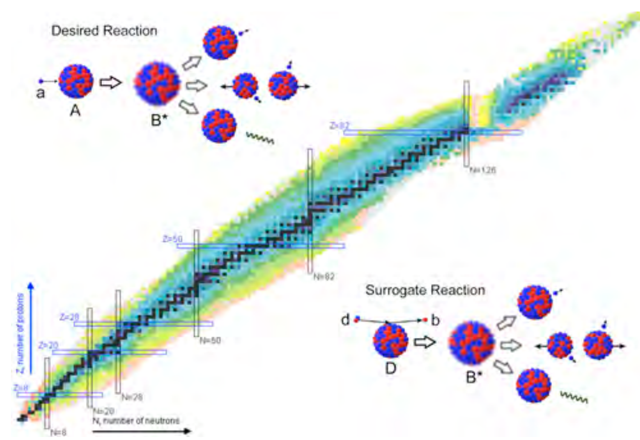


Figure 2. The National Nuclear Data Center chart shows isotopes color-coded by half-life. For the stable isotopes, in black, direct neutron-induced reactions are typically used to determine cross sections of interest. Most radioactive nuclei (decreasing isotope half-lives are shown in blue through pink) require indirect methods such as the surrogate reaction. In this technique, the same excited nucleus created by neutron capture (the "desired reaction" shown in the upper left) is produced and studied using the "surrogate reaction" shown in the lower right that is experimentally accessible. The radioactive isotopes near stability can be studied at accelerator facilities today and many additional exotic radioactive isotopes will be readily available at the Facility for Rare Isotope Beams currently under construction.

# Stewardship Science Academic Programs

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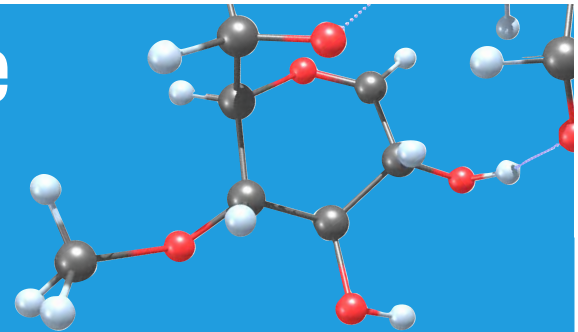
National Nuclear Security Administration

# Computational Science Graduate Fellowship



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

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Department of Energy National Nuclear Security Administration

# Stewardship Science Graduate Fellowship

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.

**BENEFITS**

- $36,000 yearly stipend
- Payment of full tuition and required fees
- $1,000 yearly academic allowance
- Yearly conferences
- 12-week research practicum
- Renewable up to four years

**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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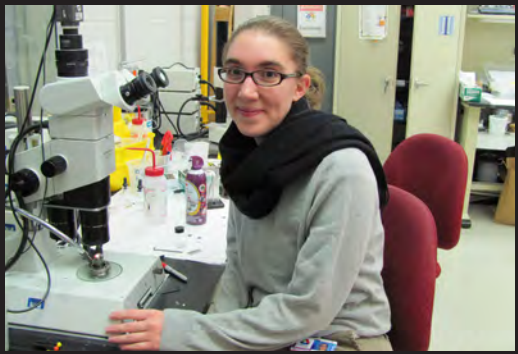

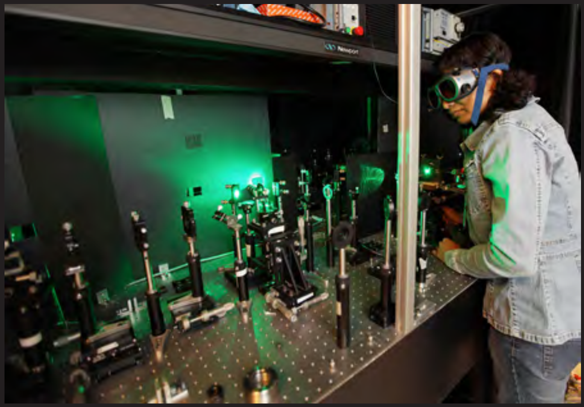

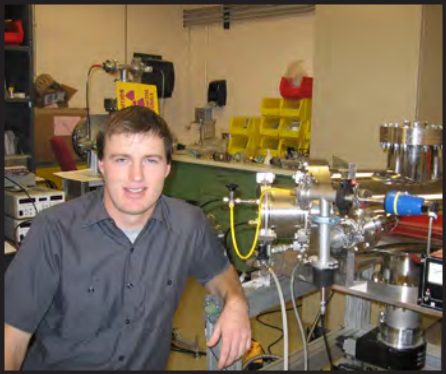

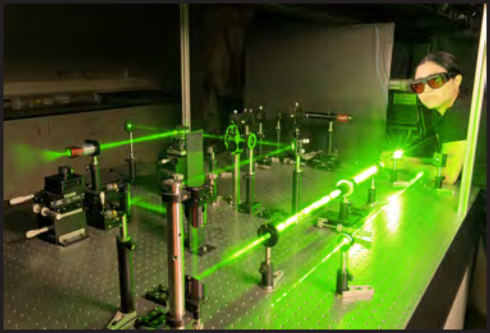

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