STEWARDSHIP SCIENCE

The SSGF Magazine 2012-2013

LASER DAYS

One fine summer at Livermore's National Ignition Facility

Sandia: Thriving with uncertainty

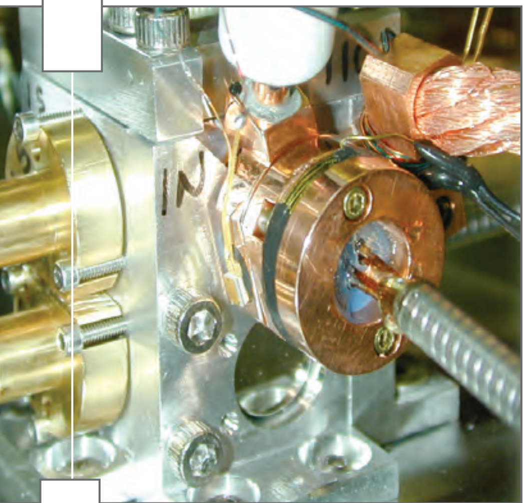
Los Alamos: Mesoscale's moment

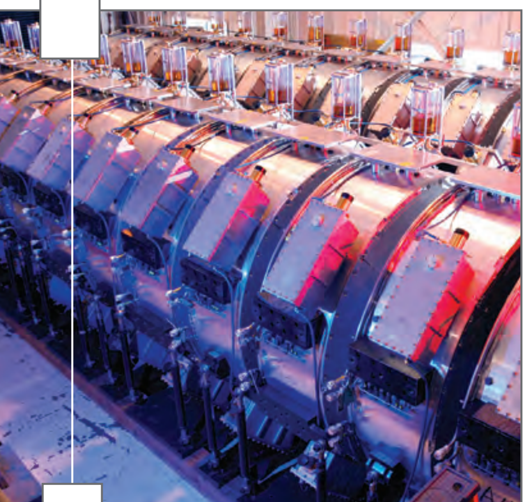
Plus: A talk with NNSA defense programs deputy Donald Cook, stewardship science fellows on location, new ideas about icy planets and a sandwich no one would want to eat

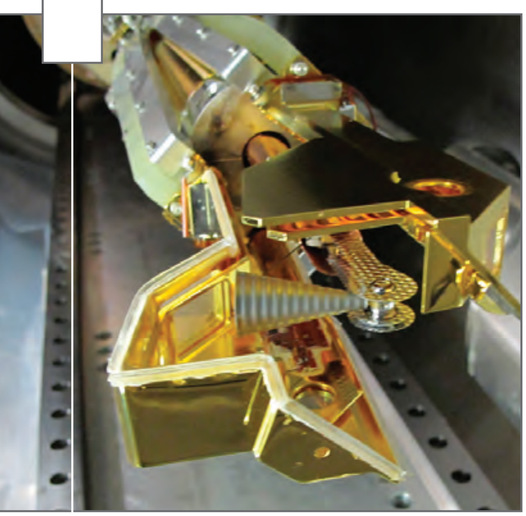
STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

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 either Lawrence Livermore National Laboratory, Los Alamos National Laboratory or Sandia National Laboratories.

BENEFITS

- **$36,000 yearly stipend**
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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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IMAGES

TOP: At Sandia National Laboratories, high magnetic fields on the aluminum side of this magnetically launched aluminum/copper flyer drive it into diamond targets at tens of kilometers per second, generating enormous pressures and shock waves in the diamond.

MIDDLE: Circular aluminum structures create magnetic fields in Los Alamos National Laboratory's Dual Axis Radiographic Hydrodynamic Test accelerator, focusing and steering a stream of electrons.

BOTTOM: A "keyhole" target for a shock timing experiment is positioned on the ignition target insertion cryostat in the cryogenic target positioning system of the National Ignition Facility at Lawrence Livermore National Laboratory.

Images courtesy of respective laboratories.

FOR MORE INFORMATION

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National Nuclear Security Administration

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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.

Christopher Deeney

Our People: The Basis for Everything We Do

IN 1942, the best scientific minds joined the nation's best project managers to develop a technology that brought a rapid end to the war. Throughout the Cold War, a pipeline of talent flowed to the nuclear weapons complex to ensure peace through a very, very hair-trigger time in history. Now, we have an equal challenge: to sustain and modernize the stockpile while providing options in arms control, stockpile reductions, counter-proliferation and non-proliferation. This challenge can be met by exceptional scientists and engineers. The Stewardship Science Graduate Fellowship (SSGF) is about these people.

America's "insurance policy," as Donald Cook terms our deterrent efforts ("Conversation: A Nightmare Deterred," page 9) is comprised of several key pillars, the first of which is our people. SSGF is a central mechanism by which we maintain this pillar. Newly minted physicists should consider his sage advice and be open to unexpected career trajectories. The formula for success is found in hard work, combined with an appreciation of the essentials of gathering data, challenging and validating codes and developing an appreciation for cutting-edge experiments.

The experiences of students Kristen John and Michael Hay, SSGF fellows who each conducted a research practicum at Lawrence Livermore National Laboratory, demonstrate this notion ("Laser Days of Summer," page 10). Kristen's work at the OMEGA laser facility on material flow under extreme shock has given her a new skill set in computer simulation of radiation hydrodynamics, assisting researchers who are conducting one-of-a-kind experimental work and gaining insights that have reshaped her dissertation topic. Likewise, Michael's work on target design is provoking laboratory researchers to consider new ideas about how mix between the capsule's outer shell and its hydrogen fuel affect the ignition threshold factor during National Ignition Facility implosions. Of his SSGF experience, Hay explains that "this is the stuff you read about in textbooks, and I'm seeing it play out in real time." I hope you enjoy reading more about their summer excursions in this edition of *Stewardship Science*, as well as learning about the strides other National Nuclear Security Administration-funded researchers are making in mesoscale science, uncertainty quantification and predictive simulation.

Christopher Deeney
Assistant Deputy Administrator for Stockpile Stewardship
U.S. Department of Energy National Nuclear Security Administration

FEATURES

COVER

A SEASON ON TARGET

This is the laser's-eye view of experiments at the National Ignition Facility (NIF) as light enters the hohlraum, which holds a BB-sized capsule containing frozen hydrogen fuel. If all goes well, X-rays that the beams generate will compress the capsule to about 100 times the density of lead, igniting atomic fusion and releasing tremendous energy. NIF, at Lawrence Livermore National Laboratory, was the focus of summer practicum projects for two Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship recipients. Princeton's Michael Hay studied capsule design physics. Caltech's Kristen John worked on simulating NIF experiments that subject materials like iron to extreme pressures and strains. Their story begins on page 10.

Stewardship Science: The SSGF Magazine showcases researchers and graduate students at U.S. Department of Energy National Nuclear Security Administration (DOE NNSA) national laboratories. Stewardship Science is published annually by the Krell Institute for the NNSA Office of Defense Science's Stewardship Science Graduate Fellowship (SSGF) program, which Krell manages for NNSA under cooperative agreement DE-FC52-08NA28752. Krell is a nonprofit organization serving the science, technology and education communities.

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A Petaflops Confidence Booster

Sequoia, the IBM Blue Gene/Q supercomputer now coming on line at Lawrence Livermore National Laboratory, will rev up the Stockpile Stewardship Program's ambitious effort to simulate conditions of the nation's aging nuclear weapons and ensure their reliability and sustainability.

"This substantially advances the pace of progress and allows the program to estimate the performance of weapons systems with vastly increased confidence," says Michel McCoy, head of Livermore's Advanced Simulation and Computing program and deputy director for computation.

By the time it begins its classified work in January 2013, Sequoia will execute 24 different weapons-system calculations simultaneously, each as large as the maximum output of Purple, a now-retired Livermore supercomputer. The designers of the new IBM machine, now rated as the world's fastest, estimate it will operate 20 to 50 times faster than Dawn, the interim Blue Gene/P Livermore researchers are using to prepare applications for Sequoia.

"Accurately quantifying the margins and uncertainty in our stockpile stewardship calculations is essential in our quest for 'predictive simulation,'" McCoy says. "A primary mission of Sequoia will be to run many simultaneous large-scale simulations of the physical systems of weapons in the stockpile. The information gained from running many similar calculations, each slightly different, allows designers to assess a weapon's robustness and search for issues."

Before it begins that classified work, researchers at Livermore and the other two national security laboratories, Sandia and Los Alamos, will use Sequoia's massive brainpower for open science. These calculations will demonstrate, for instance, how brawny supercomputers can model such complex and changeable systems as the human heart.

Flip from back cover to see movie. Story on page 19.

Whereas Dawn calculates at a maximum speed of 500 trillion floating point operations per second, or teraflops scale, Sequoia will run in the petaflops range of up to 20 million billion operations per second. The TOP500 organization benchmarked the Blue Gene/Q at 16.32 petaflops, about two-thirds faster than the former fastest computer,

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FELLOWS ON LOCATION

A key part of a Stewardship Science Graduate Fellowship is the research practicum at a National Nuclear Security Administration national laboratory. These stories recap the practicum experiences of SSGF's 2012 outgoing class.

BIG LASERS, BIG SHOCKS

Imagine being thrown into the deep end of the proverbial swimming pool for the first time. That's how fellow **Richard Kraus** would feel as he embarked on his 2010 practicum, predicted an official at **Lawrence Livermore National Laboratory's** Jupiter laser facility.

Kraus, a doctoral candidate at **Harvard University**, supervised or carried out virtually every aspect of two experiments on Livermore's powerful Janus laser, including proposal, design, execution and analysis. His goal was to understand phase transformations during shock and release, similar to conditions found in planetary impact events. The targets for his work, supervised by materials science and technology scientist Damian Swift, were two of the most common substances on Earth: quartz and water (as ice).

The research is important, Kraus says, because quartz is an abundant mineral in the planet's crust and is used as a shock-compression standard. Yet predictions for its critical point temperature – when the liquid-vapor phase boundary ceases to exist – range from 5,000 to 13,000 Kelvin.

The ice experiment was designed to explain a characteristic shape of impact craters on icy planetary bodies. Kraus had planned to use the two-dimensional velocity interferometer system for any reflector (VISAR) to image the velocity field behind a divergent shock wave in ice samples, but problems with the targets and the cryogenic system stymied his efforts.

The silica experiments were designed to determine the mineral's liquid-vapor curve and critical point by shocking it into a supercritical fluid state and releasing to the liquid-vapor phase boundary. Kraus measured shock wave velocities and post-shock temperatures for quartz samples pinged at pressures from 1 to 3 megabars. For some tests, a lithium fluoride window was placed downrange to infer the

continued on page 7

Squeezing Water, Crunching Numbers

In one small step for planetary physics – and an important one for stockpile stewardship science – Sandia National Laboratories' Marcus Knudson and colleagues have shown that water is far less compressible than previously thought.

The results, garnered from Sandia's Z machine accelerator, could force planetary scientists to recalculate the makeup of Uranus and Neptune and exoplanets – ones outside the solar system – similar to them. The findings also are a critical addition to validating the use of first principle-based models in weapons simulations.

In recent years, astronomers have discovered a new class of exoplanet that falls between the sizes of Earth and Neptune. One of the key questions is what these exoplanets are made of, a critical factor in identifying potentially habitable ones.

Planetary scientists model distant planets based on densities obtained from the combination of observed exoplanet radius and mass. These models, however, depend heavily on our understanding of the behavior of key planetary materials such as hydrogen, helium – and water.

"Our results show that water's about 30 percent less compressible than planetary scientists thought and than predicted by models currently used to estimate exoplanet composition," says Knudson, the Sandia lead on the research project. "These results question science's understanding of the internal structure of ice-giant planets and should require revisiting essentially all the modeling of these planets within and outside our solar system."

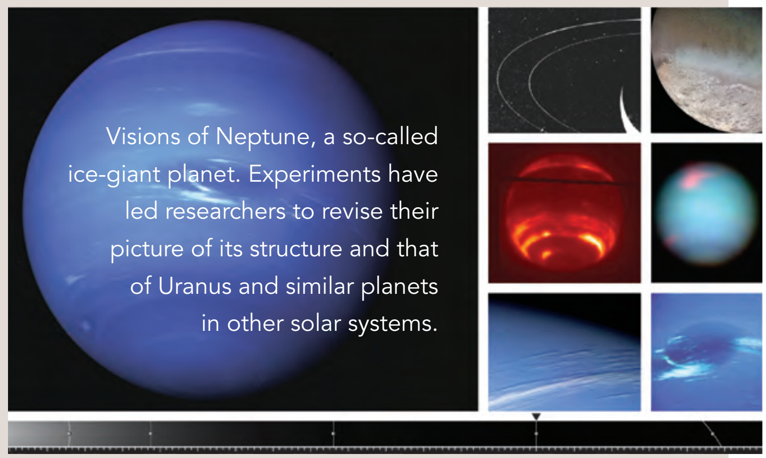
Knudson, with a team from Sandia and the University of Rostock in Germany, reproduced the interiors of giant, watery planets light years away in a space no bigger than that of a dime in the Z machine. The accelerator is one of the world's most precise tools for the study of shock physics and to test materials in conditions of extreme temperature and pressure.

The experiment harnessed Z's magnetic fields to shoot minute aluminum plates 40 times faster than a rifle bullet into a tiny water sample a few millimeters away. The impact of each plate created a powerful shock wave that compressed the water to roughly one-fourth its original volume. The shock wave then rebounded from the back of the water container, creating the equivalent of a density gradient, momentarily producing conditions similar to those throughout the interior of giant planets.

Besides finding out that water is more rigid than previously thought, the researchers also discovered that at planet-interior pressures water is in a plasma phase.

"The term 'ice giant' is a bit of a misnomer," Knudson notes. In a plasma state water also behaves as a weak metal, a fact that might help explain magnetic anomalies associated with Neptune and Uranus.

Knudson was inspired to do the experiment by the controversy over his Sandia and Rostock colleagues' first-principle equation of state



Visions of Neptune, a so-called ice-giant planet. Experiments have led researchers to revise their picture of its structure and that of Uranus and similar planets in other solar systems.

(EOS) model of water. It works directly from quantum mechanical equations to emulate water's physical properties in relation to extreme changes in temperature, pressure and volume.

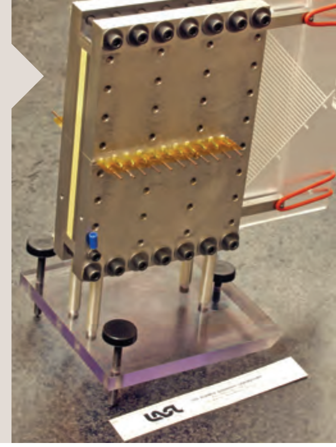
The Sandia and Rostock EOS model predicted that water is significantly less compressible under the temperature, density and pressure conditions of a planetary interior than predicted by the current models planetary scientists use.

"The experimental (results) are in excellent agreement with density functional theory predictions (of the EOS model)," the authors conclude in an article published in *Physical Review Letters*.

First principle-based models are increasingly crucial to stockpile stewardship simulations in regimes such as fusion plasmas, in which experimental testing isn't possible, Knudson explains. "In many cases using first principle models is the only way that we're going to be able to get a handle on the high energy and pressure characteristics in stockpile stewardship simulations."

- Jacob Berkowitz

This Sandwich Bites Back



A typical setup for the LANL detonation sandwich, with the yellow edge of a slab of PBX-9502 visible on the left side. The wires on the right are on the detonator and the translucent plastic is a line wave generator that begins detonation of the slab in a line. Connections for a row of timing pins are visible on the center of the steel confining material.

A sandwich recipe is helping scientists chip at the fine details of explosive detonations. The detonation confinement sandwich test – or just the detonation sandwich – explores how explosive shocks interact with their surroundings, particularly the materials confining them, says Daniel Hooks, Los Alamos National Laboratory team leader for high-explosive single crystal growth and characterization. In the region of physics the tests explore, computer simulations largely rely on theory and extrapolation of experimental data. The explosive experiment could provide data to refine or replace those estimated parameters.

Los Almos scientists Larry Hill and Tariq Aslam designed the experiment. It puts a slab of explosive material (often PBX-9502, which is used in nuclear weapons) about 6 inches square and a third of an inch thick between two plates of confining material. Detonation begins on one edge of the explosive and flows across the sandwich to the opposite edge, producing hot, rapidly expanding gases. A series of pins measures the detonation rate. At the far edge of the explosive material, a sensitive, high-speed light-streak camera records the detonation breakout shape and the shock in the confining slabs.

How the detonation shock rebounds from the constraining material "can influence the reaction front, especially in cases of the safer explosives, where the reaction takes a while," Hooks says. "That interaction with surroundings can affect things significantly."

The process is difficult for computers to model. Detonation moves faster than the speed of sound, as reactions convert solids to gases. Scientists don't fully understand the detailed chemistry, and it takes huge computing resources to capture the reactions with sufficient detail.

"Part of the point is that the model was predicting some funny stuff," Hooks says. Experiments testing those predictions are in progress, "but what we're observing so far is sort of simpler behavior."

If the confining material is heavy, like tantalum, the explosive shock pushes it away at an angle, and the shock in the confining material trails the detonation front. But "we're looking at different explosives and how they interact with different confiners of interest," Hooks says. The focus is on combinations that will stretch theoretical predictions, such as when the speed of sound in the confining material is faster or slower than the detonation front.

For instance, predictions say that when the speed of sound in a confining material is comparable to the explosive, as in aluminum and PBX-9502, the shock in the confiner keeps pace with the detonation front and may even lead it. If the experiment shows less of an impact on the front than predicted, Hooks says, "we might zoom in (computationally) to see if there's an effect that's smaller than we thought" that's influencing the outcome.

- Thomas R. O'Donnell

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the 10.51 petaflops Japanese K built by Fujitsu. To achieve Sequoia's 20 petaflops performance, the IBM Blue Gene/Q design enlists 16 compute cores per processor, up from four in the Blue Gene/P. Sequoia has 98,304 processors and 1.6 million cores. Kim Cupps, who leads Livermore's Computing Division, says the 96,000 nodes linked via Sequoia's innovative architecture will allow for "unprecedented scalability," meaning all those processors will communicate with each other especially rapidly and efficiently as they create scientific simulations.

All this hardware is arranged in 96 racks occupying about 4,000 square feet, an area that would fill a large house. But in the face of its high petascale output, IBM's designers have made Sequoia "the most energy-efficient high-performance computation platform on the planet," McCoy says. That's because its processors will operate at relatively lower frequencies to keep energy demands low. All the while, McCoy adds, Sequoia's architecture will compensate for slower processor speeds by aiding processor communications to avoid traffic jams.

- Monte Basgall

Flip from back cover to see movie. Story on page 19.

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density profile of the vaporizing silica. A line VISAR measured the velocity at the interface of the shocked, expanding silica and the LiF window.

The silica tests, Kraus says, produced plenty of data on silica release states, including post-shock temperatures and LiF interface velocity profiles, which were used to infer an average density in the vaporizing silica. Kraus planned to analyze the data and compare it to numerical models and, with colleagues, submit the experimental technique and results to the *Journal of Geophysical Research*.

Kraus' approach to the quartz tests and the data he gathered will be useful for planning future studies, Swift says. Kraus also developed a systematic approach to aligning components and laser beams that will help avoid future misalignments.

The practicum research and techniques Kraus learned will contribute to his doctoral research with advisor Sarah Stewart, which focuses on melting and vaporization during planetary impacts. But the real impact on his career may have been learning what it takes to plan and carry out a multiweek experiment on a large laser.

FROM SPLITTING TO FUSING

In a way, **Jordan McDonnell** opted for research a little lighter than his doctoral studies when it came time for his 2010 Livermore practicum.

McDonnell's research at the **University of Tennessee, Knoxville**, usually focuses on theoretical calculations of fission, which involves actinides and other heavy nuclei. When he joined **Livermore's** Nuclear Theory and Modeling group to work with advisor Erich Ormond, McDonnell chose to research calculations of nuclear fusion, which involves light nuclei like those in the hydrogen isotopes deuterium and tritium (DT). But the real effect on his career was an extension of capabilities that Ormond and his fellow scientists expect to use in projects.

At Livermore, McDonnell worked on calculating aspects of the DT fusion reaction. Although DT fusion has been extensively investigated experimentally, tests have had difficulty probing the particle interactions in the process at low energies. A first-principles theory is needed to extrapolate and evaluate experimental data in the appropriate energy range.

McDonnell worked with the research group's no-core shell model in tandem with its renormalization group model. The latter describes the internal nuclear structure and the collision between two light-ion nuclei. He eventually added to the approach by deriving the formal mathematics to describe the scattering of polarized clusters, such as deuterium nuclei, from polarized target nuclei. Previously, the group's methods could calculate only a single polarized proton or neutron scattering from a non-polarized target. Ormond says the group would use McDonnell's development – including computer code implementing it – when studying the role polarization may play in thermonuclear reaction rates.

The summer represented a considerable change for McDonnell, whose doctoral studies under Witold Nazarewicz focus on benchmark calculations of fission observables to help develop a universal energy density functional for *ab initio* predictions of nucleon interactions. Although the practicum momentarily took him in a direction different from his doctoral project, McDonnell says it was worth it. The experience let him see the broader context for his work, and the break from his usual project rejuvenated his research skills.

THEORY IN PRACTICE

In his 1923 Nobel Prize lecture, physicist Robert A. Millikan famously said, "Science walks forward on two feet, namely theory and experiment." SSGF recipient **Paul Davis** put a shoe on one of those feet during his practicum at **Sandia National Laboratories'** New Mexico campus in summer 2010.

Davis deals chiefly with experiments in his doctoral research under advisor Roger Falcone at the **University of California, Berkeley**. Using the Janus laser at nearby Livermore, Davis probes the behavior of electrons in the hydrogen isotope deuterium under warm dense matter (WDM) conditions. WDM is believed to be similar to some states of matter inside giant planets. It's also an intermediate stage of inertial confinement fusion, with characteristics lurking at the border between condensed matter and plasma physics. Davis uses X-ray scattering diagnostics to study deuterium's ionization dynamics and electron transport properties under compression and heating conditions similar to those inside the planet Jupiter. (See "Heavy Hydrogen Under Pressure" sidebar in "Diamond Soup," Stewardship Science 2010-11.)

For his summer at Sandia, however, Davis largely set aside experimentation. Working with computational physicist Michael Desjarlais, he dove into learning molecular dynamics density functional theory (DFT) calculations – giving Davis a theoretical tool to compare against his experiments.

DFT calculates the arrangement and interactions of electrons in atoms and molecules, breaking materials into geometrically arranged repeating cells to capture the material's bulk properties. Once Davis mastered the technique, he used it to calculate the dielectric and structural properties of shocked hydrogen and compared the data to results from his Livermore X-ray scattering experiments.

The theoretical work taught Davis about the physics of shocked hydrogen, including the origins of dielectric and transport properties in WDM, Desjarlais writes in an evaluation. Davis used what he learned to begin developing analytical tools for interpreting X-ray scattering experiments. Davis' research, Desjarlais adds, also helped Sandia researchers identify theoretical steps needed to improve their own analysis of X-ray scattering experiments.

COLLIDING INTERESTS

Patrick O'Malley looks at how heavy nuclei are created. During his 2009 practicum at **Livermore**, he studied ways to better understand how they come apart.

Flip from back cover to see movie. Story on page 19.

The centerpiece of the **Rutgers University** doctoral student's project with advisor Mike Heffner was the time projection chamber (TPC), a tool for detecting and identifying high-energy particles from nuclear fission and atomic decay. TPCs are used in accelerator facilities to track the products of high-energy collisions. They can help resolve uncertainties about nuclear cross sections for different nuclear materials, allowing for more precise nuclear power plant designs and better understanding of materials important to stewardship science. (See "Fission in a Small Package," Stewardship Science 2010-11.)

Heffner's group studied using a TPC to detect fast neutrons from special nuclear materials – radioactive elements such as plutonium, uranium-233 or uranium enriched in isotopes U-233 or 235. A TPC has an advantage over other detectors because it can provide information about the direction of a particle source with only a few neutron-atom collisions. That's because the TPC is insensitive to gamma rays from background radiation and nuclear fission.

Heffner and his colleagues commissioned a new TPC during O'Malley's practicum and took data from it with a neutron source in various lab locations. O'Malley worked on improving data analysis software and on calibrating gain using a combination of neutron and alpha particle sources. The calculations will help researchers determine the energy of neutrons the TPC detects. He also worked on understanding how shielding affects detection efficiency.

At Rutgers, O'Malley has worked with advisor Jolie Cizewski to study nucleosynthesis, the creation of heavier elements in the Big Bang and by stars throughout their life cycles. In particular he's looked at the nuclear shell structure for unstable isotopes and the production of elements heavier than iron. In experiments at Oak Ridge National Laboratory, O'Malley and Cizewski have aimed a radioactive ion beam at solid plastic targets in which regular hydrogen has been replaced with deuterium. The deuterium transfers a neutron to the beam, ejecting a proton. The proton's characteristics provide clues about the neutron's energy and other qualities.

There is a connection between the practicum and his doctoral research, O'Malley says. He'd calibrated gain for silicon detectors at Oak Ridge, but applying those skills to a TPC was more complicated. And since his main research involves developing plastic scintillation neutron detectors, the practicum helped familiarize him with that task's difficulties.

– Thomas R. O'Donnell

CONVERSATION

Donald L. Cook

NNSA Deputy Administrator for Defense Programs

A NIGHTMARE DETERRED

When you got your Ph.D. at the Massachusetts Institute of Technology, did you consider that you'd end up as a top administrator in a federal national-security science agency?

I thought I'd go into nuclear engineering – that would be 1970, well before Three Mile Island. I was at the University of Michigan, in the first bachelor's-level nuclear engineering graduating class. It had five people. Then I fell in with a rowdy crowd of physicists and decided to go into the part of nuclear engineering that was plasma physics. So I got into MIT. Afterward, I had a number of job offers and going to a national lab was the most attractive. I was particularly drawn to the pulse power work in its early days at Sandia because of the electrical energy the machines could harness. Limited understanding of plasma physics turned out to be one of the key limitations – and still is – in high energy density science, as we now call it. I've also done a few odd jobs. After 28 years at Sandia, I had the unique opportunity to go to England from 2006 to 2009 to head the Atomic Weapons Establishment of the United Kingdom.

You've spoken frequently about the 'deterrence mission.' What got you thinking about deterrence and what are the main components of that mission?

The Cuban Missile Crisis happened when I was just 14. I saw my parents cry before the television for three nights. They thought America was going to be attacked. That woke me up about nuclear weapons. My thinking is that nuclear weapons have made the world unsafe for unlimited large-scale conventional war. As for the deterrence mission, there are four aspects. The first is people. Second is the stockpile itself. Third is our infrastructure for R&D, engineering, manufacturing – all the bits that provide the core element of the deterrent capability besides the people. The fourth is our business practices.

Can you talk about priorities in stockpile stewardship and the national and international context that serves as a backdrop for stewardship science?

We have confidence in the existing stockpile. It is safe. It is secure. It is reliable. But our concerns are that in time it will degrade. We must modernize in an appropriate way the entirety of America's nuclear deterrent. By appropriate I mean with a real focus on safety and security. We don't have any new military requirements or aspire to new capabilities. But our stockpile is the oldest and smallest since the Eisenhower administration. I interact with many well-intentioned people. There's one view that modernization will cause proliferation, it's not in America's interest, and if we do modernize, that makes it more likely these weapons could be used and therefore would be used. I have an opposite view: America's nuclear deterrent provides not only the insurance policy for America but also for 31 or 32 other nations – the extended nuclear deterrent – and every one of those nations is absolutely watching what we're doing. If they hear nothing, they will assume we're letting these things rust. They need to know the credibility of America's nuclear deterrent is maintained and will deter aggression.

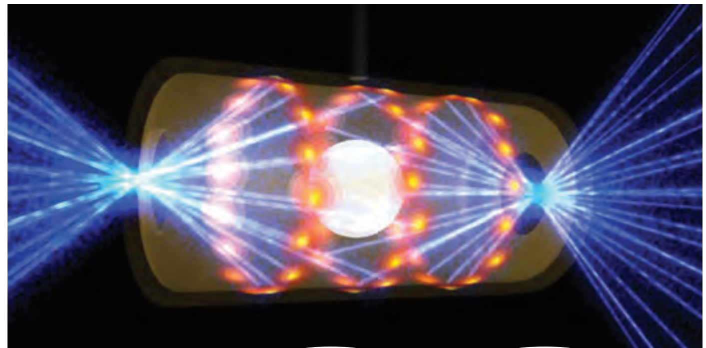
> *Think of the long shadow, about your children's grandchildren.*

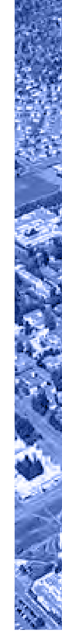
How do workforce-development programs like the Stewardship Science Graduate Fellowship further the deterrence mission?

SSGF addresses the core issue of the first element on that deterrence mission list: the people. That's the basis for everything else we do.

What's your advice to a newly minted science Ph.D. in high energy density physics, nuclear science and materials under extreme conditions who is considering a career in stewardship science?

Learn to understand the central importance of gathering data, to challenge codes and validate codes, and develop an appreciation for experiments. Think of the long shadow, about your children's grandchildren. Learn deterrence theory, read widely and don't try to plan your whole career. If you're good and you apply yourself and stay focused and don't give up and work through the challenges, your career will take care of itself. The most successful people don't worry about their careers. They have great drive to solve some of the nation's toughest problems, and we've got a fleet of those.





LASER DAYS OF

POWERFUL LIGHT SOURCES AT LAWRENCE LIVERMORE NATIONAL LABORATORY – INCLUDING THE NATIONAL IGNITION FACILITY – DRAW TWO STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP RECIPIENTS FOR A SEASON OF RESEARCH.

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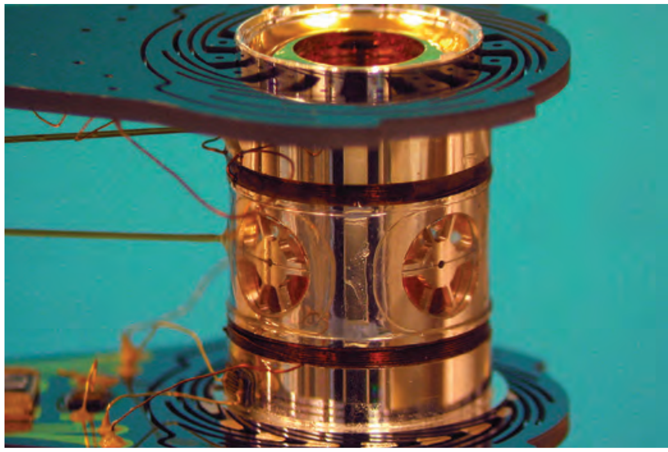
Thomas R. O'Donnell, senior science editor, has written extensively about research at the DOE national laboratories. He is a former science reporter at The Des Moines Register.



BY THOMAS R. O'DONNELL

SUMMER

Clockwise from opposite page: National Ignition Facility's (NIF) target chamber, 33 feet in diameter. Artist's conception of how NIF's lasers converge in a hohlraum, which holds a capsule containing frozen deuterium-tritium. Lawrence Livermore National Laboratory, home to NIF. A hohlraum.

LAWRENCE LIVERMORE NATIONAL LABORATORY SPREADS BENEATH VINEYARD- AND WIND TURBINE-DOTTED HILLS IN NORTHERN CALIFORNIA. There's a lake and winding roads and sidewalks. Scientists and other employees move from building to building. For longer trips, many of them ride lab-provided bicycles.

Like a university, the lab's halls and laboratories are quiet sanctums of study into materials science, biological pathogens, applied mathematics, computational science and other subjects.

No college, however, can claim the world's most powerful laser facility, a few of the world's fastest computers and a concentration of classified nuclear weapons research. Armed guards man the gates. Visitors must be cleared and many must have escorts.

Not far from one of those gates, Edward Teller, famed father of the hydrogen bomb and a driving force behind the lab's creation, kept his first office. Nearby is Building 314, a boxy, two-story former barracks dating back to the facility's roots as a World War II Navy pilot training base. This is the summer 2011 home of Stewardship Science Graduate Fellowship recipient Michael Hay, here to calculate configurations for tiny fusion energy targets.

On the other side of the sprawling complex is Kristen John in Building 381, which, though a non-classified facility, is nonetheless secure. Staff and visitors must go into a vestibule, swipe a pass and key in a code for entry. It's more modern than where Hay works, with an atrium and small stream that spills into a pool with a soothing burble. But her office is just as humble: a cubicle in a common area. John spends little time here at first; for many weeks, she's been on the other side of the country, in New York state, squeezing in as many laser experiments as possible into each day.

Hay and John are in Livermore for research practicums, required as part of their Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF). The summer experience yanks doctoral candidates from academia and thrusts them into the collaborative culture of one of four DOE laboratories. (The others are Sandia National Laboratories, which has locations in New Mexico and California, and Los Alamos National Laboratory.) For Hay, a plasma physics student at Princeton University, the practicum is an interesting side trip to his main research. John, who studies at the California Institute of Technology, has come to learn new science and possibly push her dissertation in a new direction.

Hay is primarily a theorist. John largely concentrates on experiments. Each of their summer projects connects to

Livermore's National Ignition Facility (NIF). More than 12 years in the making, NIF is designed to trigger, in a BB-sized capsule of frozen hydrogen isotopes, inertial confinement fusion or ICF – conditions like those inside stars and exploding nuclear weapons. The facility also generates powerful X-rays, creating pressures like those found in weapons, supernovae and the cores of supermassive planets.

FEATS OF STRENGTH

John is working with physicist Hye-Sook Park and Bruce Remington, group leader for material dynamics in NIF's High Energy Density Experiments program, on how materials behave under high pressures and strains. She uses computer codes called HYADES and ARES, which simulate radiation hydrodynamics, to study the flow of materials under extreme shocks. "The idea is to predict what you're going to see in the experiments and to help design the experiments," John says. "With the code you can play around with thicknesses and materials and different things, to design your experiment and help to see what's going to happen."

John has practiced her new skills by focusing on earlier experiments to quantify the strength of vanadium, used in chemical piping and as a steel additive, and tantalum, a dense metal for armor plating and projectiles. Strength is essentially resistance to deformation, but it's a radically different – and difficult to measure – quality under high pressures and strains, Park says. Theorists have made predictions, but "nobody else is experimentally studying that other than us." If the pressures NIF and other large lasers generate were to hit all at once, the target material would heat past the melting point. But most of Park's experiments ramp up the pressure over a period of nanoseconds, Remington says, "so we're studying plastic fluid flow in the solid state." Materials "actually flow plastically, so it's like a fluid with enormous viscosity."

Using powerful X-rays, the researchers record radiographic images of Rayleigh-Taylor instabilities (RTI) at the interface between the laser-powered shock and the metal target. RTI occurs when a fluid pushes into a denser fluid. The stronger the material, the less instability grows. RTI has implications for ICF because X-rays must compress the fuel capsule symmetrically, like squeezing a balloon from all sides without letting part of it push out, to ignite a thermodynamic burn. Experiments on tantalum and other elements may help to suggest ways to suppress or stabilize RTI, assuring symmetric compression.

Besides tantalum, Park, Remington and their colleagues have tested the strength of beryllium, copper and vanadium under pressure, comparing results each time with the theoretical conclusions computer simulations generate. "We've been through this with four different materials and with confident theorists every time," Remington says, "and we've never failed to set people back on their heels" with surprising results.

Flip from back cover to see movie. Story on page 19.

Park already is performing some tantalum strength tests on NIF using a ramped pressure drive. She'll conduct tantalum Rayleigh-Taylor (TaRT) NIF experiments within a year. Until then, TaRT has gone on the road to the University of Rochester's OMEGA and OMEGA EP lasers. John has been helping with so many experiments

Michael Hay

Kristen John

that she's been away from Livermore every other week for the first part of her practicum.

Hay's longest lab trips, meanwhile, are across the lab's campus for meetings. His supervisor, Larry Suter, oversees the Hohlraum Dynamics Group in Livermore's Theory and Target Design Division. A hohlraum is a gold cylinder the size of a pencil eraser. In an ICF shot, it holds a capsule containing the frozen hydrogen isotopes deuterium and tritium (DT). Rapid pulses of 192 intense laser beams enter ends of the hohlraum, creating X-rays that instantaneously burn off the pellet's plastic shell. If all goes well, the jet-like force of the burning shell will compress the isotopes to a density 100 billion times that of Earth's atmosphere and heat them to more than 100 million degrees Celsius, fusing their atoms and, if all goes right, achieving ignition – generating more energy than went into the shot.

Hay's practicum focused on that tiny shell. Like John, he uses a radiation hydrodynamics code – in this case HYDRA – to see how capsule design tweaks affect the implosion. Unlike John, Hay has experience with the code.

One of his projects examined how mixing between the burned-off outer shell and the hydrogen fuel affects ignition threshold factor (ITF). ITF weighs the roles of fuel shell velocity, the mix of ablated shell material and fuel, and other properties that affect an ICF shot's quality. "It's the amount of kinetic energy you have in a given implosion relative to the minimum you need to get ignition," says Dan Clark, a Livermore physicist who researches target design – and whose doctoral advisor at Princeton, Nathaniel Fisch, also supervises Hay. The higher the ITF, the more likely the implosion will achieve ignition.

IMPROMPTU PRESENTATION

By early August, Hay is ready to present results to the weekly group meeting, and Suter and Clark are at Building 314 for a preview. The visit quickly becomes a miniseminar as the researchers occupy a cluttered conference room. "This is good practice for your Ph.D. orals," Suter jokes.

At least five input terms influence ITF, Hay says as he writes the equation and draws a rough capsule schematic on one of the lab's ubiquitous white boards. To get at how mix affects ITF, his model held all the inputs steady except the collapsing shell's velocity and the mix fraction.

The calculations show "really, really fast shells – high velocity – they have a lot of margin. They can tolerate a lot of mix," Hay tells his small audience. "Really slow shells that are just barely igniting, they need all the fuel to be clean." Collapsing the shell with a higher velocity could overcome the damaging effects of mix, Suter notes. The problem is, higher velocity also can generate more mix.

"What you're saying is if we could get 25 percent more kinetic energy – and right now it's an issue – but if you could get 25 percent more kinetic energy, then we would be robust against lots of mix?" Suter asks.

Hay nods. "At least more mix than we thought – to the extent that you trust this mix model." Later in the summer, Hay finds the model produced mix in a way that didn't compare well with experiments. He runs a new model before heading back to Princeton. The numbers await analysis.

In a second project, Hay is examining the physics of symmetry capsules, or symcaps. These plastic stand-ins for hydrogen targets can calibrate NIF radiation drive symmetry. Symcap data help validate radiation hydrodynamics codes.

On the outside, symcaps are similar to fuel capsules. But whereas a fusion target has a layer of frozen deuterium and tritium, a symcap has a plastic layer of the same mass. Because the plastic layer is denser than DT, it's also thinner.

Symcaps usually are imploded in a series of four laser pulses with spacing and power levels similar to those used to implode DT capsules. "So a natural question," Hay says, "is what happens if you try to design laser pulses that will compress a symcap perfectly?" His early calculations show "those pulses are very different because DT targets are a lot thicker, so the shocks behave differently. They go at different speeds" because of the differences in density.

DT targets are difficult to make, so researchers hope to use symcaps for most tests, Suter says. "Mike has shown what a few people suspected: that it's just not the same."

"It's not even close," Hay laughs. "You need to start at square one and put your 'I'm designing a target from scratch' hat on."

Despite his target design work, Hay is more interested in analyzing NIF shots than in seeing one. Nonetheless, he's thrilled to contribute to the experiments. "Just a week after I got here they shot the very first DT capsule," Hay says. "This is stuff you read about in textbooks, and I'm seeing it play out in real time."

TAKING THEIR BEST SHOTS

John's practicum has launched her doctoral research on iron, the next material to undergo high-pressure studies. There are plans to test iron on NIF, but because early experiments will be on OMEGA it's important that she learn how things happen at Rochester.

Planning an OMEGA experiment takes months, including building targets at Livermore or another facility, John says. Each tiny sample is attached to an armature, boxed in plastic and bubble wrap, and treated like an infant in arms on the plane trip east.

Shot day lasts up to 14 hours. "We always bring doughnuts and coffee in the mornings and bagels and cookies and snacks in the afternoon to keep the OMEGA people happy," John says. The goal is to make as many shots as possible, "so you're working all day to make sure you're ready to go for the next one." With luck, researchers can do as many as eight in a day.

NIF is designed to implode polished capsules like this one, each 2 millimeters in diameter and filled with super-cooled deuterium-tritium fuel.

The Livermore team, including a principal investigator (often Park), postdoctoral researchers and interns, occupies a conference room next to the laser control room. Lights flash, there's a countdown, and it's over in nanoseconds. The researchers check data flooding in from instruments and prepare for the next shot. At the end of the day they gather other results, including radiographic images, before getting some sleep for the flight back to Livermore, where the real data analysis begins.

Observing laser experiments is an unexpected course for John, who earned her bachelor's degree in aerospace engineering at the University of Texas at Austin. At Caltech, she planned to research fracture mechanics under Guruswami Ravichandran, but the practicum has offered an opportunity to explore a new topic – and to establish a partnership.

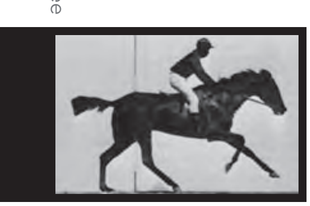
"It was fortunate that we had Kristen and the SSGF because we had wanted to collaborate with this (Livermore) group for quite a while" through Caltech's Predictive Science Academic Alliance Program (PSAAP) center, Ravichandran says. NNSA sponsors five PSAAP centers to develop, validate and verify large-scale simulations of processes of interest to the agency. Caltech's center studies the physical processes that occur when hypervelocity objects strike metals.

Ravichandran and fellow Aerospace Engineering Professor Michael Ortiz, the center's director, have visited Remington, Park and others at Livermore to discuss collaborating.

"The first productive step was when Kristen came up here to spend a summer to see what we do," Remington says. John's support from the DOE NNSA SSGF, Ravichandran says, made it possible.

SEEKING IRON INSIGHTS

Iron has been a staple material for centuries, but there's still much we don't know about it, Remington says, because high-pressure experiments have become available only in the last couple decades. When researchers have put iron under pressure, they've "found it's more complicated than they thought – by a large measure."



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Iron's crystal structure changes at relatively low pressures, and its strength may differ based on its crystal phase.

"But no one knows," Remington says. At the kinds of pressures NIF can achieve, "it's never been done. It's not been modeled that way." Ortiz, meanwhile, has led researchers from Caltech, Stanford and Princeton universities in developing a multiscale model of stress-induced phase transformations in iron. The Livermore experiment, Ravichandran says, "would be a good platform to validate some of those models" and Livermore researchers are eager to test them.

Since returning to Caltech, John has begun designing iron OMEGA experiments, which are tentatively scheduled for July 2012. "My practicum is very much tied to what I'll be doing for my thesis," she says, but it had little in common with her previous research.

"A lot of physics is new to me so there's been a high learning curve there." When John wasn't at OMEGA, she was reading papers and talking with colleagues. Her cubicle's location made it easy to connect with others. "I can go to almost anyone, even someone I've only maybe met once or twice, and ask him or her questions."

Hay credits his immediate comfort at Livermore to an earlier experience at nearby Lawrence Berkeley National Laboratory while earning his bachelor's degree at the University of California, Berkeley, and at the Princeton Plasma Physics Laboratory. At Livermore, "people are usually eager to work with me and you can walk down the hall and find an expert in just about anything. It's a really unique environment. I want to make a career out of it."

First, though, Hay must finish his doctoral research on the physics of stimulated Raman scattering, a phenomenon in which atoms and particles interact with laser light, altering its direction and wavelength. SRS research has implications for a number of fields, including hohlraum physics.

Remington and Park, meanwhile, already are lobbying John to return to the lab as she concludes her doctoral research. "Finish your classes," Remington says, turning to John, "because I have every intention to just keep you here." SS

CALCULATING THE UNKNOWN

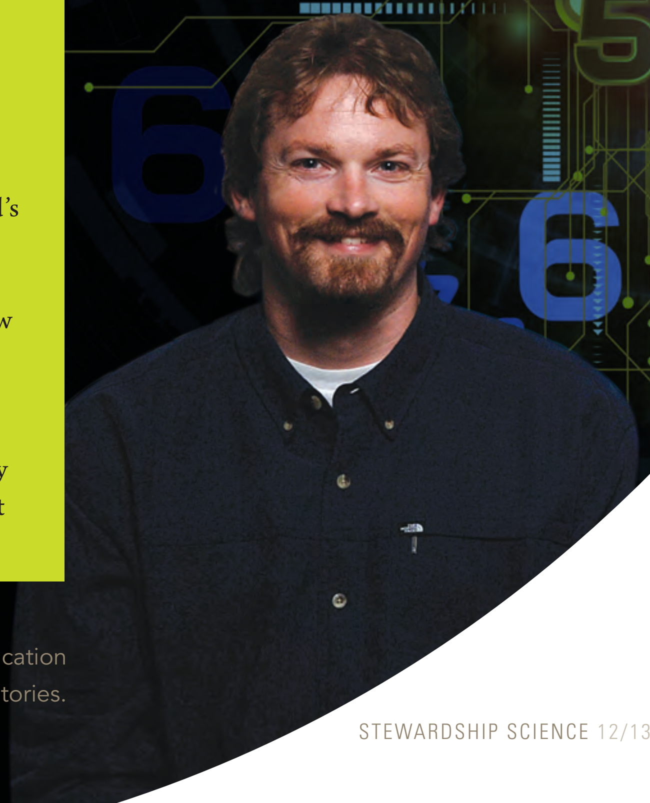
BY JACOB BERKOWITZ

HOW MUCH FAITH CAN WE PUT IN THE PREDICTIONS OF STEWARDSHIP SCIENCE MODELS? UNCERTAINTY QUANTIFICATION AIMS TO FIND OUT.

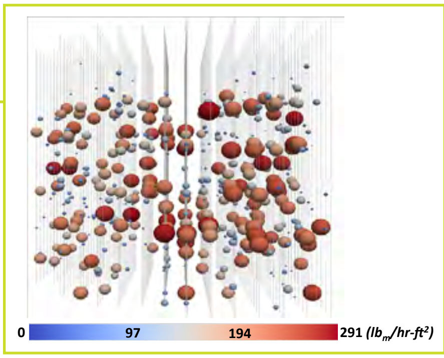
EVERY YEAR, THE PRESIDENT OF THE UNITED STATES RECEIVES A REPORT THAT ATTESTS TO THE SAFETY AND RELIABILITY OF THE U.S. NUCLEAR WEAPON STOCKPILE. The Stockpile Stewardship Annual Certification and Report is the written equivalent of a two thumbs up from each of the directors of the Department of Energy's Sandia, Lawrence Livermore and Los Alamos national laboratories.

But what's increasingly at the heart of the certification and report is something the president doesn't know. Neither do the weapons lab directors or even the scientists and engineers on the front lines of the world's most sophisticated and extensive nuclear weapons management program. They have a name for this missing information: the new field of uncertainty quantification (UQ).

Today, one of the most important frontiers of stockpile stewardship science is about clearly knowing and quantifying the effects of what you don't know.



Mike Eldred leads an uncertainty quantification team at Sandia National Laboratories.



Uncertainty analysis can help scientists understand physical processes like those taking place inside a nuclear reactor core. Here, in a quarter-core section viewed from the side, vertical lines indicate fluid-flow channels. Spheres represent localized boiling, their colors echoing boiling rate – lower for blue and higher for red. Sphere size varies based on degree of uncertainty.

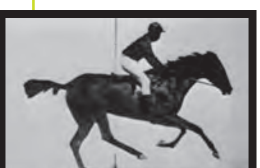
"The field of uncertainty quantification is experiencing an extremely rapid growth," says Mike Eldred, who's pioneered stockpile stewardship-related UQ research for the past decade at Sandia's New Mexico campus. "The presence of UQ in research calls has gone from minimal a decade ago to today, when you have a hard time finding a call that doesn't have a significant emphasis on UQ. There's a lot of competition for post-docs who have experience in this field."

WHY UNCERTAINTY NOW?

The emphasis on UQ results from the move from underground testing to supercomputer simulations as a cornerstone of the U.S. Stockpile Stewardship Program.

"If you're going to rely on simulation models you need to assess their predictive accuracy," notes Eldred, a distinguished member of the technical staff in Sandia's Optimization and Uncertainty Quantification Department within the Computation, Computers, Information and Mathematics Center. "How faithful are they in terms of representing reality?"

UQ is a mix of statistics, computer science and a vein of pure logic that would be at home amid a huddle of ancient Greeks parsing the nature of what's knowable with Socrates. The key is that UQ isn't just about errors in a simulation's math or physics. UQ's also about identifying and quantifying the fundamental sources of uncertainty – whether in the underlying physics or models – that if propagated through a simulation might significantly skew predictions. In essence, UQ aims to enable stockpile stewardship scientists to provide precise statements about their degree of confidence in their simulation-based predictions.



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Jacob Berkowitz is a science writer and, most recently, author of The Stardust Revolution: The New Science of Our Origin in the Universe *(Prometheus Books, 2012).*

Eldred says getting a handle on what we don't know in stockpile stewardship has never been more important than now. As weapons age, simulations increasingly rely on extrapolated predictions, ones that simulate far beyond the support of available full-system experimental data.

Asked about this, Eldred pauses. "Well, that's the key challenge we're facing. It's a very daunting problem. You have some historical test data. You don't have the ability to do additional tests, or if you do they're very expensive; you can't test directly in the regime where you need to make a prediction. So what do you do? You work hard to make that computational simulation as good as it can be by grounding it in data where you have data. But you still have to make this leap of faith in the extrapolatory case. It's one of the most challenging things that we have to do within Stockpile Stewardship."

This is where UQ comes in. It's the critical component in determining just how big that leap of faith is – actually giving it a number that can inform risk-based decision making.

UQ has its roots in DOE's Accelerated Strategic Computing Initiative (ASCI), established in 1995 to support simulation and modeling in stockpile stewardship. ASCI initially focused on adapting existing computational techniques to new, massively parallel-processing supercomputers. Now known as the Advanced Simulation and Computing (ASC) Program, its success has led to the emergence of new core issues related to advanced applications of predictive science. UQ is a key one of those.

ASC "recognized that UQ was important all along, but they had to get their ducks in a row in terms of the parallel simulations first," says Eldred, who joined Sandia in 1994 after completing a doctoral degree in aerospace engineering from the University of Michigan. "This is a common situation. It doesn't make a whole lot of sense to do design optimization and UQ using computational models if the computational models aren't ready for it."

ADDING IN UQ

Computer gamers judge a new game by comparing the virtual experience with reality. For example, does a virtual car behave like a real car? For gamers, the answer is an intuitive and visceral one. For those responsible for the nation's nuclear stockpile, it's a much more difficult assessment.

"One important objective of UQ is to make the intuitive notion of confidence mathematically sound," Stanford University UQ expert Gianluca Iaccarino told a computer science conference in 2009.

Since models can't be compared directly against the launch, delivery and detonation of a nuclear weapon, the degree of confidence the stockpile stewardship program can provide about the accuracy of its simulations and predictions relies on the trio of techniques known as verification, validation (known collectively as V&V) and UQ, also known as quantification of margins and uncertainty. This trio of techniques is a "significant unifying challenge to stockpile stewardship," the *2012 Stockpile Stewardship and Management Plan* reports.

Verification is the process, initially developed in engineering sciences, of ensuring that a computer code is in fact solving equations correctly. Validation asks a question not of the math, but of the underlying physics; it assesses the accuracy and applicability of the physical models used in the code. Neither of these directly addresses UQ (although UQ is often part of the validation process).

Even if a simulation's math and underlying physics are correct, there can still be significant model uncertainties that will appreciably affect a simulation's predictions, Eldred explains. That's because uncertainties are inherent to factors that go into any model – such things as materials parameters or variable boundary conditions in temperature, pressure or radiation.

Over the past decade, UQ science has matured into a sophisticated analytical field, and one of its bedrock facts is that uncertainty comes in two basic flavors: aleatory and epistemic.

Aleatory uncertainties are those that result from the inherent physical variability in a system. In stockpile stewardship, this type of uncertainty arises from inconsistency in material properties, such as manufacturing tolerances of new components and the rate of aging-related changes. Though this kind of uncertainty is unavoidable, it can be modeled within a probabilistic framework based on observed data. In other words, it's possible to define the uncertainty and propagate the associated probability information through a model.

Epistemic uncertainty is more slippery and challenging, Eldred says. It comes from a lack of knowledge and is reducible given the opportunity to collect more information. For example, there are a half-dozen turbulence models stockpile stewardship scientists can use to simulate warhead atmospheric re-entry. Which is best

UQ PLUG-AND-PLAY

One of the Sandia group's key goals is to lower the bar for adoption of uncertainty quantification methods by making their UQ programs plug-and-play easy for end-users.

"There's a cultural evolution that's had to take place," Mike Eldred says of the past decade, as the modeling end-users have become familiar with interfacing UQ with their codes.

Part of the challenge is that Sandia's Optimization and Uncertainty Quantification Department works directly with Sandia's Verification and Validation Group in the Engineering Sciences Division, but not as directly with the stockpile stewardship modelers. Thus it's all the more important that the UQ algorithms and codes be simply integrated with stockpile stewardship models.

A big step in this direction has been the Sandia UQ group's development of DAKOTA (Design Analysis Kit for Optimization and Terascale Applications), an open-source software toolkit that provides a delivery vehicle for much of the UQ research at the DOE defense laboratories. Originally designed in the late 1990s to address design optimization, DAKOTA now also provides a variety of UQ methods so that modelers can address the question: *How much confidence do you have in your answer?*

Though DAKOTA is a major step in making UQ user friendly, Eldred would like to continue to remove overhead from the process of integrating it with stockpile stewardship simulations.

Eldred envisions analysts who are comfortable using a given simulation capability "to do UQ as part of their existing processes with a minimum of additional setup. We're trying to make it easier and easier to use so that it can become ingrained in how we do business."

WANTED: SCIENTISTS SEEKING UNCERTAINTY

Sandia's uncertainty quantification team hasn't yet played practicum host to a Stewardship Science Graduate Fellowship recipient, but Mike Eldred is looking forward to that day.

He and colleagues welcome anyone interested in the growing field of UQ, which will become ever more important as supercomputing scales up the complexity of scientific simulations.

A practicum isn't the only option for the UQ-curious, Eldred adds. "Sandia's Computer Science Research Institute sponsors an active visitor program, supporting summer students, faculty sabbaticals *and* practicum visits."

to use? The answer is an epistemic uncertainty that generates additional spread in the possible range of simulation results.

Different application areas can have divergent mixes in terms of aleatory and epistemic uncertainty. For example, Eldred works on a DOE Office of Science project applying UQ to wind energy simulations. The wind turbine simulations involve mostly aleatory uncertainty (inherent physical variability rather than a lack of information) and there's a relative wealth of real-world data.

"That's unheard of in a stockpile stewardship context," Eldred says. "Stockpile stewardship tends to be more information-poor, and the uncertainty tends to be more epistemic. Where you have very limited information UQ is used to give you a sense of the range of what's possible. When that range contains a situation that is undesirable, then this indicates the need to invest additional resources to more accurately characterize the uncertainties."

As a result, during the past decade Eldred and others in the stockpile stewardship program have been pioneers in developing and finessing UQ in a data-poor, epistemic context.

One of the keys has been developing algorithms that effectively track and differentiate between aleatory and epistemic uncertainties so their various contributions can be assessed in pegging a simulation's overall UQ.

They've also had to do this in the context of another finite limit: money. Eldred says that given the enormous expense of running large day- or week-long simulations on teraflops- or petaflops-capable computers, "the name of the game in UQ is being able to efficiently and accurately compute the statistics that you need using as few computational simulations as possible."

His group has focused on ramping up efficiency of UQ algorithms. "Instead of on the order of a hundred thousand simulations, for example, we can exploit certain features of the solution, and we might only require tens of simulations to get a UQ result of comparable or better accuracy. That's been the big payoff for the research investment. And when there is a mixture of aleatory and epistemic sources, the savings can be further amplified."

Flip from back cover to see movie. Story on page 19.

Eldred's team is now working to improve the UQ programs' ease of use and efficiency. One of the keys to improving efficiency in UQ algorithms: developing ones that include on-the-fly sensitivity analysis and error estimation. This is the ability to identify the dimensions and regions within the input parameter space that contribute the most to overall uncertainty and automatically shift computational resources to model these in higher resolution.

"We need to have algorithms that on the fly can figure out where important things are happening in the multidimensional, stochastic input space and focus there while providing less resolution elsewhere."

PUTTING QUEST TO THE TEST

Achieving these next-generation stockpile stewardship UQ algorithms will be aided by cross-fertilization through the new DOE Office of Science UQ institute named QUEST, for Quantification of Uncertainty in Extreme Scale Computations. The program includes scientists from Sandia and Los Alamos national laboratories and from four universities.

QUEST has its work cut out for it, Eldred says. "There's a significant amount of complexity that we have to deal with, including multifidelity, multiphysics, and multiscale issues. There are a lot of challenges in terms of being able to deal with the variety of simulations and a variety of levels of modeling within a typical weapons system, including coupling between components, from small parts to the integration of sub-systems."

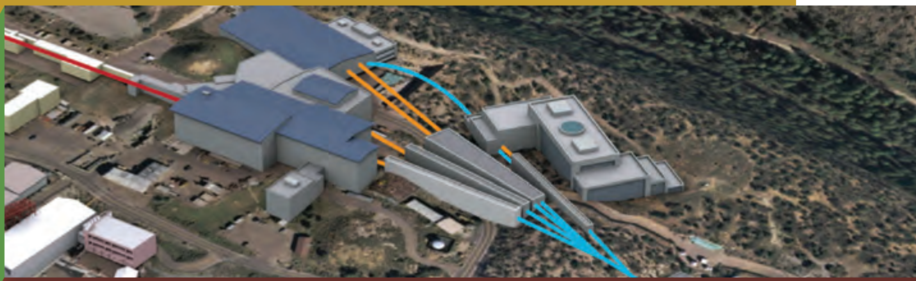
Recent history in other applications has shown that UQ is as critical for risk-informed decision-making as it is for predictive simulations. As such, UQ not only is an increasingly critical piece of ensuring the safety and reliability of the nuclear weapons stockpile. It also will answer key public policy questions.

As a 2011 DOE-led UQ workshop noted: "Science-based predictive modeling and simulation are playing an increasing role in supporting political policy decision-making. … Global climate change, and the roles played by, for example, the global climate models and integrated climate impact assessment models are a key exemplar of this type of interaction between the computational science community and the world at large."

In providing the essential UQ science that underpins the stockpile certification and report that the president receives, Eldred and other leading UQ researchers are making good on the age-old aphorism that it's the wise man who knows what he doesn't know. SS

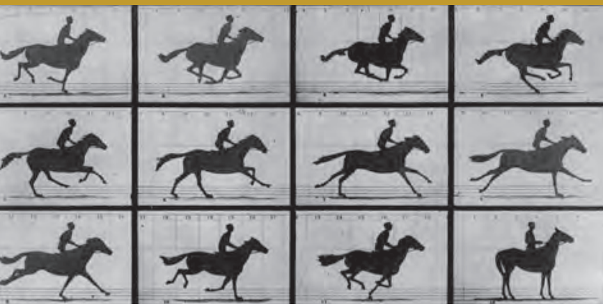
WORKING FOR MESOSCALE

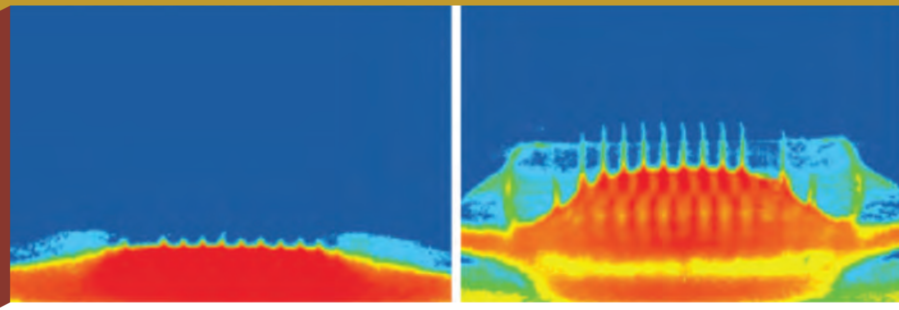
BY KARYN HEDE



Left: X-ray laser flashes generated in an undulator, an arrangement of magnets that directs high-energy electrons. **Right:** Artist's-concept aerial view of the proposed MaRIE facility at Los Alamos National Laboratory.

LOS ALAMOS SCIENTISTS STUDY THE MICROSTRUCTURE OF MATERIALS WHOSE BEHAVIOR IS CRUCIAL TO STOCKPILE STEWARDSHIP. TO FURTHER THAT RESEARCH, THEY'VE PROPOSED MARIE, THE MATTER-RADIATION INTERACTIONS IN EXTREMES EXPERIMENTAL FACILITY.





MATERIALS SCIENCE HAS A BORDER PROBLEM. Combined with advances in physics and molecular modeling, the discipline has made huge strides in deciphering how materials behave at the atomic and nanometer scales and, at the other extreme, bulk. But little is known about microstructure, the scale from microns barely visible to the unaided eye up through millimeter-sized samples large enough to pinch between the thumb and forefinger. This scientific frontier – the unknown middle between atomic and bulk scale – dwells in the mesoscale.

'In the real world nothing is perfect and pristine nor perfectly homogeneous.'

"If you want to make the transition from observing materials to being more predictive, you've got to cross this micron frontier," says John Sarrao, program director of the proposed Matter-Radiation Interactions in Extremes (MaRIE) experimental facility at Los Alamos National Laboratory.

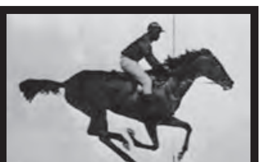
Crossing from uncertainty to mesoscale science would let scientists predict, for example, the stability of composite explosives based on solid experimental evidence. The dynamic processes most important for national security occur on a microseconds scale with materials both dense and irregular. Capturing the dynamic activity of exploding or imploding materials requires instruments that sample processes at picosecond intervals. Until recently, the tools that measure mesoscale events like shock waves propagating through materials haven't existed.

That's why the development of the free-electron laser (FEL) has generated excitement among physicists and materials scientists.

Richard Sandberg, a physicist at Los Alamos, says the free-electron laser has revolutionized the kinds of experiments scientists can conduct to probe matter's behavior. Specifically, the Linac Coherent Light Source (LCLS), the world's first hard X-ray free-electron laser, at Stanford's SLAC National Accelerator Laboratory, already has demonstrated that short-pulse lasers can provide beautiful atomic snapshots of biomolecules in motion.

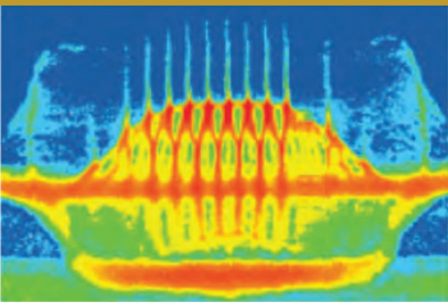
The LCLS generates X-rays a billion times more intense than other synchrotron light sources, which also use electron accelerators to generate X-rays. The difference, Sandberg says, is that the light from most X-ray sources isn't coherent, akin to the diffuse light from a flashlight. The FEL generates coherent photons – uniform packets of light that all travel together in a narrow beam. These uniform and predictable beams make FEL X-rays perfect for probing structure on the atomic scale. But perhaps most important, these coherent X-rays can be tuned to pulse on femtosecond (10^{-15} second) intervals, short enough to capture dynamic action happening on the atomic scale.

Flip from back cover to see



movie. Story on page 19.

Karyn Hede is a freelance journalist whose work has appeared in Science, Scientific American, New Scientist, Technology Review *and elsewhere.*



Far left: Eadweard Muybridge's still frames of a horse in motion, from which he made a short film of the animal running. **Left:** Researchers have proposed using the MaRIE facility to use X-ray pulse technology called coherent diffraction imaging (CDI) and, seen here, proton radiographs to capture series of stop-motion snapshots and string them together to show motion. Proton radiographs enlist magnetic lenses to focus scattered protons on a detector to create images like these frames depicting ejecta on a shock-loaded surface. CDI records the pattern of coherent X-rays as they scatter off the sample, then reconstructs a high-resolution image via computer algorithm, with no lens involved.

X-RAYS WITH HORSEPOWER

In essence, an FEL can create action movies whereas earlier technology could only capture before-and-after snapshots. The X-ray pulse technology is similar to the way a photographer uses a high-speed flash or shutter to capture a series of stop-motion snapshots that when strung together create a movie. The result is like a digital-photo flipbook. When you thumb through the pages, a short movie materializes before your eyes, Sandberg notes, much like Eadweard Muybridge's famous seconds-long film made from a series of stills of a running horse.

One proposed technique for the MaRIE facility is coherent diffraction imaging (CDI), which is under rapid development across the world. In CDI, images are captured with a charge-coupled device (CCD) similar to the technology used in digital cameras. Unlike a traditional camera, in which the digital image is projected through a lens, CDI records the pattern of the coherent X-rays as they scatter off the sample. It then reconstructs a high-resolution image using a computer algorithm, all without using a lens.

"This technology is a major advance for several reasons," Sandberg says. "Now the resolution of your images, or how fine of details you can see, is not limited by the quality of your lens. Also, these powerful X-ray pulses can actually damage the sample, destroying it as it records the images.

"It's also going to damage any optics used. If you did have a lens it could get destroyed, and these precision optics are very difficult to manufacture, very expensive lenses. So this coherent diffractive imaging is an ideal mating of technique with the development of the source of X-ray free electron lasers."

Because of its low X-ray energy, though, the FEL at Stanford is limited to imaging materials primarily composed of lighter elements, such as carbon in biological samples or low-molecular-weight metals such as aluminum. Many of the materials of interest for national security, such as iron, uranium and plutonium, have high densities (often called "high Z" for their high atomic number). In addition, Sandberg says, the material samples will need to be thicker, requiring a shorter-wavelength, higher-energy photon to penetrate them.

Until recently, trial-and-error experimentation has dominated materials science. Bulk-scale experiments have advanced understanding of how materials behave en masse. We know, for example, how stresses affect various metals and how they will behave from extremely cold temperatures to melting points. At the opposite extreme, atomic-scale measurements have advanced nanomaterial manufacturing.

Likewise, within the realm of national security there is an urgent need to move away from observation and validation of material performance toward accurate prediction and control.

Mesoscale science addresses these very issues. It offers clues about how impurities affect crystal formation and how the resulting structural deformations affect behavior in bulk-scale materials under working conditions. It deals with how grain size, voids and interfaces in composite materials influence that material's function. These mesoscale problems turn out to be critical for predicting the behaviors of composite explosives and the nuclear weapons stockpile and for addressing other top national security scientific priorities. In addition, mesoscale science is expected to contribute substantially to improving manufacturing processes, thereby allowing much more predictable and reliable products.

"In the real world nothing is perfect and pristine nor perfectly homogeneous," Sarrao says. "There are defects and voids and interfaces and wrinkles, and in fact it's those properties that determine how materials behave."

Understanding how microstructures develop in materials and devising predictive models that could guide manufacturing will require a combination of measurement tools and computational firepower.

REVEALING MOMENTS IN THE HISTORY

Scientist Wilhelm Conrad Röntgen (1845-1923) demonstrates that a new type of radiation, which he names X-rays, can penetrate materials. To generate X-rays he accelerates electrons released by a cathode (then known as cathode rays) in a vacuum tube. He also discovers a thin sheet of lead completely blocks the rays. While testing lead's ability to block the rays, Röntgen holds his thumb and index finger in their path, inadvertently creating the first X-ray images of the human body. His discoveries earn him the 1901 Nobel Prize in Physics.

Physicist Max von Laue (1879-1960) discovers X-ray diffraction using crystals. The discovery comes to him when he realizes that short electromagnetic rays, or X-rays, should cause interference when passing through a crystal. Von Laue works out the mathematics, publishes in 1912 and wins the Nobel Prize in Physics in 1914.

William D. Coolidge, (1873-1975) a physicist at the General Electric Research Laboratory, invents the Coolidge tube, a specialized vacuum tube for generating X-rays. The device, still in use today, made X-rays safe for medical diagnosis.

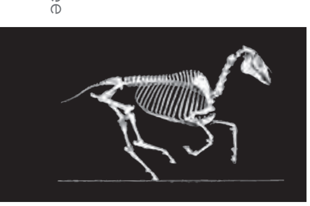
Edwin M. McMillan, (1907-1991) an American chemist, develops the first synchrotron electron accelerator facility at Berkeley Radiation Laboratory. McMillan uses the synchrotron to discover the first transuranium element.

FACILITATING STEWARDSHIP

Los Alamos proposed MaRIE in response to a National Nuclear Security Administration (NNSA) call for New Flagship Experimental Science, Technology & Engineering Facility Concepts, a long-term program for major new developments in support of NNSA's Stockpile Stewardship Program.

The MaRIE would provide experimental tools capable of probing complex structure and recording how it changes in extreme environments.

As currently envisioned, MaRIE would include the Multi-Probe Diagnostic Hall (MPDH), a multi-instrument complex that would allow, for the first time, simultaneous X-ray scattering and charged-particle imaging measurements of dense, complex materials. Instrumentation would include proton radiography and the centerpiece of the MaRIE project: the X-ray free electron laser (XFEL), a high-intensity, low-average-power source of 50- to- 100-kiloelectron volt (keV) X-rays – so-called hard X-rays, needed to penetrate dense metal samples. A kilometer-long tunnel would house the 20-GeV (gigaelectron volts, a million times more energetic than keV) electron beam. When the beam is injected into an undulator, a long series of magnets, it would emit the desired coherent X-rays that pulse in-phase on the femtosecond scale necessary to capture atomic activity.



Flip from back cover to see movie. Story on page 19.

Proton radiography, a technique developed at Los Alamos using the lab's 800-mega-electron volt (MeV) proton beam, measures micron-scale void formation in dense materials such as nuclear fuel rods. In addition, the electron linear accelerator for the XFEL is expected to be a useful electron source for high-resolution charged-particle radiography, a complement to proton radiography.

A final part of the proposal is the M4 – the Making, Measuring and Modeling Materials Facility, designed to synthesize and characterize materials on the mesoscale and to perform computational and modeling research iteratively with experimental results the instrument facilities obtain.

FIRST EXPERIMENTS

Once in place, the XFEL would immediately be used in several proposed experiments designed with input from more than 225 scientists from 80 institutions. At a series of workshops, this group worked with Los Alamos staff scientists to identify scientific obstacles to predicting materials performance in extreme environments.

The experiments fall under two broad categories, says Toni Taylor, division leader of the lab's Materials Physics and Applications Division. One set will explore dynamic materials performance. These experiments are primarily designed to better understand properties of the current nuclear stockpile and to explore how composite materials such as the high explosive PBX-9501 behave under various conditions.

OF X-RAY LIGHT SOURCES

The Department of Energy Office of Basic Energy Sciences develops a second-generation instrument, Brookhaven National Laboratory's National Synchrotron Light Source. Its X-ray ring begins operation in 1984.

Argonne National Laboratory's Advanced Photon Source (APS), the largest third-generation synchrotron, opens. Its 7 GeV electron storage ring supports 70 X-ray beam lines and provides some of the brightest hard X-ray beams in the United States. The APS is a national user facility that supports more than 3,000 experiments a year.

The Linac Coherent Light Source at the SLAC National Accelerator Laboratory becomes the world's first hard X-ray free electron laser facility. The linear accelerator-based light source provides X-ray radiation 10 billion times greater in peak power and brightness than any other such device.

In the 100th anniversary of Max von Laue's discovery, work proceeds worldwide on new X-ray free electron laser sources and high-resolution tabletop soft X-ray sources using amplified ultrafast lasers to enable coherent X-ray diffractive imaging, or CXDI.

"When you are using explosives, you don't have a single uniform crystal structure," Taylor explains. "You have a plastic-bonded explosive that is a complex composite material. The performance is complex because the material itself is complex. You want high confidence that they will perform, but you also want them to be safe. You don't want them to go off when they are not supposed to. And you also want to understand how they age."

The idea is to use the XFEL for imaging and combine it with other diagnostics, such as X-ray absorption spectroscopy, to examine the chemical state simultaneously with the dynamic state in the same facility using the same sample, a feat that is not possible with current facilities.

The second set of experiments aims to design a precise manufacturing process. Besides providing better control over materials important to national security, these experiments also would have applications across a broad range of industrial manufacturing, including innovations in clean energy and custom metal design and fabrication.

"Every vision of advanced manufacturing for innovation has the same challenge," Sarrao says. "These are the challenges that mesoscale science is designed to solve."

For example, the process of metal solidification on the mesoscale is almost entirely unknown. "There certainly are models for solidification," Taylor says, "and we are starting to do some proton radiography, but it is very much in its infancy. You really do need much better diagnostics than we have at the moment. That's what MaRIE would bring to the table."

Another of the early experiments would explore the physics of solid-solid phase transformation and defect formation. One particularly interesting example is a shock wave traveling through a polycrystalline metal. In such a sample, metal grains are typically tens of microns in diameter and each sample is expected to be about 10 to 100 grains thick, making typical sample sizes ranging from tens to hundreds of microns up to millimeters.

In this proposed experiment, a beam of hard X-rays would intercept a shock wave traveling through the polycrystalline sample and scatter off the various grains' boundaries and density fluctuations. The resulting interference pattern, captured by the detector array, would produce a series of images capable of reconstruction into high-fidelity images. Under extreme pressure, the material deforms, phase transformation takes place and damage can be tracked in real time, Sandberg says.

The experimental findings would feed into computational models to develop new predictive tools to inform the next generation of materials development. MaRIE could then help integrate atomic-level physics into predictions of bulk-scale behavior for the first time.

"The results coming out of the LCLS are generating a lot of excitement about the use of hard X-rays in the imaging community," Sandberg says. "The MaRIE facility and the proposed XFEL there could revolutionize the way people are looking at denser, high-Z materials." SS

A Plasma State of Mind

BY CHRIS YOUNG

Chris Young

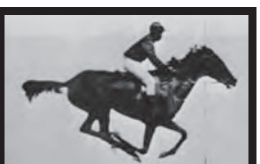
My first undergraduate research experience was right out of a science fiction movie. I had 10 weeks to build a plasma thruster. What I knew at the time about space propulsion came from the *Star Wars* trilogy, but my advisor was confident, and soon a bright purple glow emanated from a soup-can-sized device.

What I find fascinating about plasmas (not the blood kind but the fourth state of matter) is that they aren't really part of your daily experience on Earth. Sure, the sun is a plasma, and lightning is a plasma, but you can't interact with those things like you can with, say, a glass of water. Everything that's intuitive about earthly solids, liquids and gases won't help you know what plasma is and does. It's a hidden part of the universe that comes to life on Earth only in exceptional circumstances. In my case, it takes a vacuum chamber pumped down to a billionth of atmospheric pressure just to turn on the thruster.

Although improving the design of space propulsion devices is important for lowering satellite costs, the real value of studying these thrusters comes from what we learn about the plasma inside them and how we might use this knowledge to manipulate plasmas usefully. I'm working on a fundamental plasma physics problem that, besides helping determine how well the thruster runs, will generally apply to plasma devices.

Specifically, I study plasma sheaths: little electrical layers that form between plasmas and any surface they touch. Most every manmade plasma must be contained by something, and the plasma will probably touch that container in some way. Where this contact occurs, the sheath forms, so they're quite common in the world of plasmas.

Flip from back cover to see movie. Story on page 19.



We plasma physicists must worry about electrical layers because plasmas are full of tiny charged particles intermixed with all the other molecules that make up regular gases. This is why plasmas get that fancy designation as a separate state of matter. You can make a plasma from just about anything if you add enough energy to it – by heating it or running an electric current through it – so that some electrons that used to be happily attached to their parent atoms are free to roam. These newly independent electrons leave behind oppositely charged ions that are now short of a full electron set. With all these free charges flying around, a host of new physics and several new ways to make the plasma do what we want come into play. When charged particles abruptly slam into the container wall the plasma adjusts and forms the sheath, preventing its otherwise uninhibited journey through a given device.

Sheaths are found everywhere in today's plasma applications. In some cases, like using plasma to etch patterns in semiconductors, we want it to contact a surface in a precise and controlled way. You can bet there's a sheath on the semiconductor surface that must be taken into account. In other cases, like fusion reactors in which we want to create the hottest and densest plasma possible, allowing it to reach the wall can be a serious detriment. The more we understand about how sheaths work, the better we can use them to our advantage in such applications.

Plasmas could transform society.

A recent summer at Lawrence Livermore National Laboratory gave me new perspectives on how plasma physics researchers are applying their findings to critical energy and stewardship science problems. Plasmas form the heart of fusion energy research, where the challenge is getting them to stick around long enough to extract more energy than spent producing them. They also are found in nuclear explosions and are integral in determining what happens during and after detonation. Facilities like Livermore's National Ignition Facility allow unprecedented access to these extreme conditions and we are learning much about the physics at play.

Plasmas could transform society, especially in renewable energy. This is why I consider continuing research into them to be vital. I was hooked from day one in the space propulsion lab, and I plan to build a career around learning as much as possible about this intangible part of our universe.

This page samples experiences of Stewardship Science Graduate Fellowship recipients. The author, winner of this year's SSGF Essay Slam, is a second-year fellow at Stanford University.

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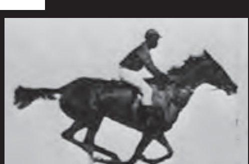
* Class of 2012. Completed program Aug. 2011
**Class of 2012. Completed program March 2012

MESOSCALE MOVIES

In the 1880s, Eadweard Muybridge assembled seconds-long films of animals in motion, including horses, made from photographs shot in sequence. Researchers at Los Alamos National Laboratory want to do something similar with X-ray pulse and other advanced technologies to create a digital-photo flipbook of how materials change under extreme conditions. These movies would reveal dynamics otherwise hidden if viewed as a collection of snapshots. For more, flip to page 19, where *Working for Mesoscale* begins.



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